

Table S1. Cartesian coordinates of the optimized stationary points involved in the reactions of **CAT** with benzene, calculated at the B3LYP/DGDZVP level of theory in CH₂Cl₂ solvent.

Names	Cartesian Coordinates			
CAT	8	-0.755969000	1.992711000	0.248868000
	46	0.222041000	0.094584000	-0.122398000
	8	-1.744675000	-1.681600000	1.409533000
	6	-2.193148000	-1.425440000	0.285160000
	8	-1.602793000	-0.660514000	-0.606459000
	6	-3.510667000	-2.003254000	-0.214785000
	1	-4.110736000	-1.235323000	-0.709655000
	1	-3.302653000	-2.786211000	-0.951486000
	1	-4.068850000	-2.436674000	0.616769000
	6	0.090629000	3.019241000	0.813541000
	1	0.681974000	2.550904000	1.599367000
	1	0.748016000	3.441219000	0.046140000
	1	-0.542962000	3.803284000	1.239821000
	6	-1.639237000	2.502039000	-0.777529000
	1	-1.057822000	2.922448000	-1.605133000
	1	-2.239244000	1.660876000	-1.120101000
	1	-2.280509000	3.272184000	-0.337420000
	6	2.539581000	-0.767831000	-0.082917000
	8	1.546746000	-1.527961000	-0.375178000
	8	2.281155000	0.463049000	0.175048000
	6	3.935189000	-1.306219000	-0.021490000
	1	4.659163000	-0.500990000	-0.158401000
	1	4.095462000	-1.758733000	0.962864000
	1	4.074481000	-2.080569000	-0.778853000
TS-1(O1)	8	-0.768214000	1.806072000	1.599085000
	46	-0.448000000	0.274789000	-0.120609000
	8	0.229457000	2.152212000	-2.189263000
	6	1.263316000	1.980222000	-1.524958000
	8	1.316683000	1.184449000	-0.482322000
	6	2.578854000	2.656761000	-1.858190000
	1	3.028086000	3.089975000	-0.960484000
	1	3.279039000	1.913007000	-2.252241000
	1	2.420850000	3.432833000	-2.609008000
	6	-2.022027000	1.782830000	2.302857000
	1	-2.803034000	1.600533000	1.566201000
	1	-2.031387000	0.985297000	3.055060000
	1	-2.181735000	2.752137000	2.789298000
	6	0.348140000	2.056069000	2.471826000
	1	0.424595000	1.272365000	3.235349000

	1	1.242587000	2.062509000	1.850297000
	1	0.220138000	3.031256000	2.956074000
	6	-2.626276000	-1.148142000	-0.841431000
	8	-1.936948000	-1.048555000	-1.877067000
	8	-2.208395000	-0.646563000	0.292054000
	6	-3.978814000	-1.819268000	-0.819883000
	1	-4.196706000	-2.237560000	0.165166000
	1	-4.746288000	-1.072994000	-1.052068000
	1	-4.019829000	-2.600444000	-1.581760000
	6	2.144056000	-2.325379000	-0.867228000
	6	0.865831000	-2.366355000	-0.287243000
	6	0.712454000	-2.119233000	1.089989000
	6	1.838474000	-1.834070000	1.879660000
	6	3.108242000	-1.796148000	1.297077000
	6	3.261201000	-2.043020000	-0.077001000
	1	2.261399000	-2.520047000	-1.930156000
	1	0.004784000	-2.629064000	-0.895132000
	1	-0.268957000	-2.198380000	1.549403000
	1	1.720873000	-1.651813000	2.944966000
	1	3.980562000	-1.579671000	1.908967000
	1	4.251635000	-2.016754000	-0.524679000
TS-1(O2)	8	0.307580000	-1.871428000	0.875165000
	46	-0.336711000	0.029729000	0.129791000
	8	-3.282742000	-0.642650000	0.632715000
	6	-2.965904000	-0.998739000	-0.508583000
	8	-1.769179000	-0.899464000	-1.036818000
	6	-3.981253000	-1.600855000	-1.476233000
	1	-4.853909000	-1.955837000	-0.925374000
	1	-4.298387000	-0.824359000	-2.180136000
	1	-3.541615000	-2.416119000	-2.055273000
	6	-0.350408000	-2.324150000	2.083617000
	1	-0.405303000	-1.469595000	2.757466000
	1	-1.354987000	-2.692209000	1.856484000
	1	0.255841000	-3.115948000	2.534232000
	6	0.483965000	-2.930684000	-0.094807000
	1	-0.486885000	-3.290830000	-0.445895000
	1	1.054370000	-2.511390000	-0.922670000
	1	1.048141000	-3.742070000	0.374757000
	6	-0.891489000	2.724050000	0.334633000
	8	-0.980751000	1.796279000	-0.587637000
	8	-0.395217000	2.513054000	1.455284000
	6	-1.461515000	4.068306000	-0.067712000
	1	-2.532384000	4.077363000	0.162208000
	1	-0.977682000	4.862710000	0.503944000

	1	-1.344316000	4.245339000	-1.139045000
	6	3.186294000	-0.085309000	-1.827602000
	6	2.454203000	0.968369000	-1.263416000
	6	2.528143000	1.214221000	0.117747000
	6	3.331809000	0.399179000	0.931271000
	6	4.061077000	-0.652830000	0.366317000
	6	3.988924000	-0.894048000	-1.013442000
	1	3.131147000	-0.272998000	-2.897080000
	1	1.837933000	1.602919000	-1.894773000
	1	1.981955000	2.045051000	0.556729000
	1	3.389870000	0.590959000	1.999891000
	1	4.685693000	-1.282044000	0.995748000
	1	4.558642000	-1.709870000	-1.452004000
INT-1(O1)	6	0.763077000	-1.947285000	-0.590596000
	6	1.981803000	-1.692944000	-1.270659000
	6	3.168762000	-1.615695000	-0.558290000
	6	3.172539000	-1.786655000	0.845262000
	6	1.990821000	-2.038788000	1.529160000
	6	0.772253000	-2.124793000	0.818635000
	1	-0.130530000	-2.165078000	-1.168042000
	1	4.112230000	-1.731274000	1.388747000
	1	1.997032000	-2.188865000	2.605049000
	1	-0.128819000	-2.452572000	1.327941000
	8	-1.296831000	2.001724000	0.624056000
	46	-0.213826000	0.051388000	0.270553000
	8	-2.301092000	-1.027810000	-1.823607000
	6	-2.684492000	-1.230944000	-0.663101000
	8	-2.005624000	-0.927463000	0.418061000
	6	-4.017552000	-1.902353000	-0.359142000
	1	-4.554404000	-1.363369000	0.425893000
	1	-4.627368000	-1.953229000	-1.262733000
	1	-3.834736000	-2.918754000	0.005188000
	1	1.975542000	-1.579827000	-2.350827000
	1	4.104757000	-1.431952000	-1.079232000
	6	-2.154907000	2.015356000	1.782174000
	1	-1.570043000	1.635018000	2.620271000
	1	-2.465778000	3.046115000	1.985249000
	1	-3.032882000	1.381577000	1.621091000
	6	-1.935001000	2.582866000	-0.535503000
	1	-2.228493000	3.612073000	-0.300386000
	1	-1.194290000	2.571710000	-1.333452000
	1	-2.816918000	1.999227000	-0.820879000
	6	1.864145000	1.850317000	-0.568552000
	8	1.182188000	2.009590000	-1.592250000

	8	1.555950000	1.041931000	0.414740000
	6	3.181369000	2.581711000	-0.352801000
	1	3.239363000	2.987417000	0.660690000
	1	4.008693000	1.874554000	-0.473521000
	1	3.288985000	3.384841000	-1.083999000
INT-1(O2)	6	1.667934000	1.522348000	0.595128000
	6	2.575899000	0.855360000	1.453457000
	6	3.646925000	0.150739000	0.920311000
	6	3.837722000	0.095187000	-0.478021000
	6	2.959206000	0.747805000	-1.334540000
	6	1.865816000	1.470195000	-0.804876000
	1	0.910102000	2.171939000	1.023143000
	1	4.685155000	-0.451819000	-0.883302000
	1	3.117143000	0.724031000	-2.409245000
	1	1.249384000	2.074343000	-1.463345000
	8	1.087538000	-1.767732000	0.073330000
	46	-0.087950000	0.017129000	-0.249191000
	8	-1.477266000	2.294951000	1.415322000
	6	-1.707683000	2.402384000	0.204958000
	8	-1.203410000	1.640309000	-0.739343000
	6	-2.653209000	3.463290000	-0.345293000
	1	-2.311382000	3.841056000	-1.311385000
	1	-3.639630000	3.010449000	-0.491759000
	1	-2.747731000	4.282322000	0.370090000
	1	2.436766000	0.917206000	2.529271000
	1	4.349727000	-0.352460000	1.579240000
	6	1.095379000	-2.686590000	-1.043950000
	1	1.321189000	-2.102096000	-1.935197000
	1	1.878358000	-3.432995000	-0.878583000
	1	0.120407000	-3.171054000	-1.147022000
	6	0.903368000	-2.444094000	1.340754000
	1	1.701282000	-3.183889000	1.459394000
	1	0.977341000	-1.685709000	2.118540000
	1	-0.078062000	-2.923476000	1.378793000
	6	-2.522863000	-1.574029000	0.181004000
	8	-2.367498000	-1.378624000	1.394250000
	8	-1.719545000	-1.162051000	-0.766718000
	6	-3.731295000	-2.335708000	-0.357169000
	1	-4.198172000	-2.912024000	0.443657000
	1	-4.459648000	-1.614823000	-0.743544000
	1	-3.448294000	-2.995068000	-1.181266000
TS-2(O1)	6	1.205403000	-1.182802000	0.007277000
	6	2.061588000	-0.974983000	-1.103287000
	6	3.444990000	-1.114455000	-0.981031000

	6	4.003770000	-1.448156000	0.261567000
	6	3.180089000	-1.656094000	1.378072000
	6	1.796957000	-1.520894000	1.251130000
	1	0.217641000	-2.015781000	-0.297195000
	1	5.081973000	-1.551584000	0.358789000
	1	3.618768000	-1.924059000	2.336112000
	1	1.161490000	-1.699858000	2.115897000
	8	-2.061719000	1.721320000	0.424341000
	46	-0.448291000	0.172930000	0.172231000
	8	-0.678616000	-2.936825000	-0.565195000
	6	-1.831432000	-2.415812000	-0.391904000
	8	-2.017423000	-1.200269000	-0.067917000
	6	-3.041358000	-3.305205000	-0.571028000
	1	-3.962996000	-2.726612000	-0.512795000
	1	-2.977649000	-3.819079000	-1.533364000
	1	-3.037244000	-4.068464000	0.212992000
	1	1.632595000	-0.722927000	-2.070081000
	1	4.088354000	-0.963431000	-1.844379000
	6	-2.970597000	1.489627000	1.517516000
	1	-2.363608000	1.298708000	2.403330000
	1	-3.582241000	2.385014000	1.675279000
	1	-3.613865000	0.627695000	1.310678000
	6	-2.745892000	2.064811000	-0.798024000
	1	-3.370679000	2.948728000	-0.626296000
	1	-1.972485000	2.289096000	-1.532254000
	1	-3.368633000	1.229313000	-1.137330000
	6	1.177086000	2.489744000	-0.414177000
	8	0.630356000	2.482600000	-1.530102000
	8	0.971605000	1.616923000	0.535270000
	6	2.204393000	3.553452000	-0.040767000
	1	2.043374000	3.911647000	0.979344000
	1	3.206528000	3.113354000	-0.082030000
	1	2.156450000	4.388061000	-0.742560000
TS-2(O2)	6	1.767771000	0.449230000	0.098892000
	6	2.296735000	0.040860000	1.345807000
	6	3.570982000	-0.525013000	1.438019000
	6	4.340852000	-0.698378000	0.278624000
	6	3.842878000	-0.292952000	-0.967908000
	6	2.569263000	0.276105000	-1.053809000
	1	1.231669000	1.678149000	0.175559000
	1	5.331768000	-1.141084000	0.347898000
	1	4.448337000	-0.417026000	-1.862604000
	1	2.196029000	0.603265000	-2.022484000
	8	0.300537000	-2.105041000	-0.195769000

	46	-0.332839000	-0.001336000	-0.207213000
	8	0.870080000	2.912471000	0.247110000
	6	-0.369024000	2.965354000	-0.058727000
	8	-1.080922000	1.945859000	-0.322082000
	6	-1.028841000	4.324864000	-0.097941000
	1	-2.035289000	4.257035000	-0.509639000
	1	-1.077524000	4.718395000	0.921945000
	1	-0.419272000	5.010875000	-0.690790000
	1	1.709380000	0.184649000	2.250846000
	1	3.966462000	-0.827638000	2.404707000
	6	0.031082000	-2.792745000	-1.438097000
	1	0.461512000	-2.189040000	-2.237225000
	1	0.516862000	-3.773717000	-1.411743000
	1	-1.047051000	-2.903482000	-1.587692000
	6	-0.112151000	-2.878943000	0.953123000
	1	0.399227000	-3.846919000	0.927959000
	1	0.190033000	-2.322161000	1.839353000
	1	-1.196616000	-3.023084000	0.951384000
	6	-3.116995000	-0.709118000	0.378639000
	8	-2.834818000	-0.475145000	1.566818000
	8	-2.278738000	-0.659528000	-0.619373000
	6	-4.540817000	-1.070724000	-0.035065000
	1	-5.108083000	-1.427620000	0.826918000
	1	-5.032675000	-0.174587000	-0.429286000
	1	-4.543685000	-1.824711000	-0.826245000
INT-2(O1)	6	1.421280000	0.592685000	0.270053000
	6	1.865777000	1.409455000	-0.782012000
	6	3.196905000	1.857379000	-0.807843000
	6	4.080568000	1.507601000	0.219204000
	6	3.632832000	0.702395000	1.274653000
	6	2.308309000	0.242413000	1.301310000
	1	1.773106000	-1.099002000	-1.139797000
	1	5.109053000	1.859640000	0.199315000
	1	4.313003000	0.427483000	2.077990000
	1	1.979372000	-0.390045000	2.123015000
	8	-2.656498000	-0.834634000	0.404682000
	46	-0.455841000	-0.089067000	0.323617000
	8	1.861282000	-2.063579000	-1.329956000
	6	0.982379000	-2.736274000	-0.592533000
	8	0.145654000	-2.189888000	0.138879000
	6	1.099937000	-4.226397000	-0.720996000
	1	2.065943000	-4.545890000	-0.318493000
	1	0.292883000	-4.713620000	-0.176282000
	1	1.072475000	-4.509553000	-1.776446000

	1	1.181130000	1.702993000	-1.573453000
	1	3.535278000	2.483777000	-1.630416000
	6	-2.974680000	-1.934109000	1.269218000
	1	-2.403341000	-1.796991000	2.188528000
	1	-4.047094000	-1.929499000	1.498469000
	1	-2.701290000	-2.889193000	0.804791000
	6	-3.384769000	-0.876228000	-0.833479000
	1	-4.462628000	-0.854182000	-0.631136000
	1	-3.092342000	0.007520000	-1.401062000
	1	-3.138774000	-1.784868000	-1.397977000
	6	-1.525999000	2.531970000	-0.424715000
	8	-1.559992000	2.094522000	-1.590944000
	8	-1.096838000	1.881237000	0.616763000
	6	-1.995768000	3.949516000	-0.105418000
	1	-2.502795000	4.389518000	-0.966177000
	1	-2.665175000	3.947304000	0.759495000
	1	-1.129632000	4.567977000	0.153221000
INT-2(O2)	6	1.666268000	-0.303495000	-0.036941000
	6	2.198054000	-0.816604000	1.156837000
	6	3.589258000	-0.903810000	1.329630000
	6	4.453220000	-0.489401000	0.309648000
	6	3.924278000	0.019703000	-0.883718000
	6	2.535946000	0.119371000	-1.055521000
	1	1.238659000	1.630567000	1.127307000
	1	5.529916000	-0.560378000	0.443228000
	1	4.589799000	0.344892000	-1.680599000
	1	2.141173000	0.528558000	-1.983510000
	8	-0.402259000	-2.390076000	0.103797000
	46	-0.325117000	-0.205422000	-0.299053000
	8	1.064521000	2.598807000	1.068301000
	6	0.266484000	2.835473000	0.030477000
	8	-0.233296000	1.941635000	-0.665752000
	6	0.027143000	4.293339000	-0.229082000
	1	-0.690319000	4.415239000	-1.038730000
	1	-0.344178000	4.770987000	0.681529000
	1	0.974427000	4.773202000	-0.492144000
	1	1.538282000	-1.158462000	1.951574000
	1	3.991545000	-1.299164000	2.259901000
	6	0.113983000	-3.274884000	-0.911156000
	1	1.072592000	-2.869712000	-1.233474000
	1	0.257129000	-4.272757000	-0.481841000
	1	-0.577286000	-3.332004000	-1.759836000
	6	-1.625727000	-2.888387000	0.686520000
	1	-1.426742000	-3.862223000	1.147630000

	1	-1.938216000	-2.168308000	1.441329000
	1	-2.403886000	-2.985375000	-0.077272000
	6	-3.228830000	0.218294000	0.290896000
	8	-2.846624000	0.447279000	1.460919000
	8	-2.458274000	-0.121801000	-0.690589000
	6	-4.712386000	0.310606000	-0.065288000
	1	-5.292815000	0.706290000	0.770757000
	1	-4.853665000	0.945651000	-0.945237000
	1	-5.089727000	-0.685570000	-0.321387000

Table S2. Cartesian coordinates of the optimized stationary points involved in the discussion on the effects of the six univalent ligands on C–H activation, calculated at the B3LYP/DGDZVP level of theory in CH₂Cl₂ solvent.

Names	Cartesian Coordinates			
TS-2-OCH ₃ (O1)	6	-1.558694000	0.334749000	0.132712000
	6	-2.138191000	0.504299000	-1.149704000
	6	-3.466636000	0.149330000	-1.400249000
	6	-4.249657000	-0.381394000	-0.365435000
	6	-3.704893000	-0.549867000	0.916556000
	6	-2.373228000	-0.205320000	1.156968000
	1	-0.915502000	1.465122000	0.524083000
	1	-5.284463000	-0.657499000	-0.555134000
	1	-4.318833000	-0.952296000	1.719072000
	1	-1.958507000	-0.343632000	2.152129000
	8	2.686647000	-1.001999000	0.036859000
	46	0.510199000	-0.256864000	0.093009000
	8	-0.458521000	2.659136000	0.728306000
	6	0.692198000	2.714539000	0.164877000
	8	1.292556000	1.697973000	-0.299284000
	6	1.340577000	4.073661000	0.031035000
	1	0.823614000	4.631793000	-0.756370000
	1	1.229187000	4.633757000	0.962128000
	1	2.394307000	3.977332000	-0.231300000
	1	-1.546500000	0.941097000	-1.952082000
	1	-3.893377000	0.288553000	-2.390840000
	6	3.011469000	-2.370335000	0.329940000
	1	2.165611000	-2.779987000	0.880592000
	1	3.157233000	-2.936049000	-0.599099000
	1	3.928769000	-2.409604000	0.930073000
	6	3.672269000	-0.366679000	-0.791956000
	1	3.750820000	-0.882140000	-1.757632000
	1	3.351330000	0.663024000	-0.941878000

	1	4.647121000	-0.384740000	-0.289426000
	8	-0.054050000	-2.111884000	0.598429000
	6	-0.621968000	-2.896225000	-0.423628000
	1	-1.607684000	-2.527301000	-0.749515000
	1	0.022350000	-2.982289000	-1.316160000
	1	-0.767152000	-3.915734000	-0.028234000
TS-2-OCH₃(O2)	6	-1.138715000	-0.992302000	0.035865000
	6	-1.793528000	-1.043714000	1.287237000
	6	-3.184672000	-1.164987000	1.379821000
	6	-3.956635000	-1.243934000	0.212229000
	6	-3.332464000	-1.211987000	-1.042444000
	6	-1.940546000	-1.091075000	-1.123577000
	1	-0.024541000	-1.844864000	-0.021668000
	1	-5.038182000	-1.337639000	0.280200000
	1	-3.929097000	-1.285991000	-1.949163000
	1	-1.468057000	-1.080796000	-2.104968000
	8	-1.001313000	1.990706000	-0.117757000
	46	0.553529000	0.409742000	-0.087966000
	8	0.815663000	-2.744600000	-0.051016000
	6	1.980086000	-2.201919000	-0.069551000
	8	2.171008000	-0.950707000	-0.072899000
	6	3.174522000	-3.125271000	-0.098016000
	1	4.102223000	-2.560031000	-0.013419000
	1	3.096937000	-3.849897000	0.716536000
	1	3.168702000	-3.683407000	-1.039084000
	1	-1.206212000	-0.997118000	2.203447000
	1	-3.666887000	-1.202847000	2.354327000
	6	-0.987221000	2.737572000	-1.353073000
	1	-1.139178000	2.018579000	-2.158889000
	1	-1.809491000	3.461593000	-1.342695000
	1	-0.027335000	3.248140000	-1.474570000
	6	-0.927601000	2.858327000	1.033024000
	1	-1.759372000	3.570840000	0.998326000
	1	-1.022647000	2.224032000	1.915136000
	1	0.029716000	3.387759000	1.046575000
	8	1.874630000	1.946440000	-0.262152000
	6	2.897823000	1.991192000	0.700087000
	1	2.521397000	2.162242000	1.725517000
	1	3.516941000	1.079759000	0.713728000
	1	3.566549000	2.835381000	0.458102000
INT-2-OCH₃(O1)	6	1.512070000	-0.346799000	-0.065053000
	6	2.266783000	-1.025689000	0.906953000
	6	3.668950000	-0.973673000	0.884459000
	6	4.335721000	-0.257161000	-0.117459000

	6	3.590831000	0.413024000	-1.095745000
	6	2.188540000	0.374315000	-1.066367000
	1	0.704544000	1.458637000	1.366491000
	1	5.422606000	-0.223191000	-0.137185000
	1	4.097403000	0.968993000	-1.882425000
	1	1.630363000	0.909850000	-1.831543000
	8	-2.852175000	-0.471479000	-0.187073000
	46	-0.502059000	-0.378024000	-0.073495000
	8	0.527244000	2.429112000	1.329822000
	6	-0.215880000	2.679014000	0.253076000
	8	-0.650532000	1.785816000	-0.485868000
	6	-0.465552000	4.137880000	0.011530000
	1	0.471855000	4.611934000	-0.296084000
	1	-1.212327000	4.263854000	-0.770906000
	1	-0.792579000	4.620705000	0.935521000
	1	1.760786000	-1.610664000	1.670103000
	1	4.239005000	-1.499321000	1.648311000
	6	-3.684235000	0.642696000	-0.528136000
	1	-3.090071000	1.314808000	-1.147161000
	1	-4.562062000	0.298792000	-1.089479000
	1	-4.016575000	1.171405000	0.375050000
	6	-3.538062000	-1.452608000	0.604941000
	1	-4.394122000	-1.852574000	0.046768000
	1	-2.812301000	-2.240149000	0.810100000
	1	-3.892977000	-1.007923000	1.544266000
	8	-0.486678000	-2.330608000	0.461261000
	6	-0.113884000	-3.264661000	-0.525324000
	1	-0.725047000	-3.200611000	-1.443416000
	1	0.944183000	-3.175709000	-0.824359000
	1	-0.252519000	-4.280469000	-0.115670000
INT-2-OCH ₃ (O2)	6	-1.308598000	-0.496312000	0.111353000
	6	-1.912453000	-1.287488000	-0.884555000
	6	-3.274973000	-1.620160000	-0.820575000
	6	-4.059183000	-1.173249000	0.249656000
	6	-3.473484000	-0.387699000	1.251113000
	6	-2.114230000	-0.049465000	1.177565000
	1	-1.255263000	1.303542000	-1.151710000
	1	-5.114052000	-1.432579000	0.302657000
	1	-4.073745000	-0.034979000	2.087736000
	1	-1.684674000	0.570089000	1.963859000
	8	1.102802000	-2.245919000	-0.236419000
	46	0.697637000	-0.080789000	0.082984000
	8	-1.236395000	2.289977000	-1.233281000
	6	-0.376876000	2.767566000	-0.338773000

	8	0.349449000	2.044838000	0.358759000
	6	-0.364123000	4.264296000	-0.241846000
	1	0.423318000	4.588734000	0.436286000
	1	-0.211108000	4.694916000	-1.235029000
	1	-1.336451000	4.609667000	0.121775000
	1	-1.320837000	-1.658260000	-1.719918000
	1	-3.719853000	-2.229268000	-1.605235000
	6	1.568587000	-2.892771000	0.965878000
	1	0.827468000	-2.692834000	1.740529000
	1	1.641403000	-3.972238000	0.790584000
	1	2.542594000	-2.490346000	1.261623000
	6	1.980276000	-2.498367000	-1.355094000
	1	2.091221000	-3.580917000	-1.484252000
	1	1.500230000	-2.069068000	-2.235559000
	1	2.950700000	-2.023536000	-1.187780000
	8	2.773265000	0.135918000	0.050757000
	6	3.352781000	1.285012000	0.600006000
	1	3.111687000	2.211106000	0.043943000
	1	3.061822000	1.465052000	1.653616000
	1	4.454921000	1.190510000	0.592702000
TS-2-NH ₂ (O1)	6	1.601948000	0.186665000	0.062532000
	6	2.269291000	-0.178390000	1.260199000
	6	3.600794000	-0.603696000	1.257363000
	6	4.303675000	-0.685667000	0.046874000
	6	3.675119000	-0.330499000	-1.155573000
	6	2.345117000	0.098685000	-1.143324000
	1	0.969257000	1.388336000	0.177089000
	1	5.339339000	-1.017737000	0.041061000
	1	4.223758000	-0.385140000	-2.093117000
	1	1.875569000	0.388984000	-2.081239000
	8	-2.671452000	-1.191236000	-0.125640000
	46	-0.472558000	-0.396913000	-0.091505000
	8	0.570753000	2.606396000	0.250705000
	6	-0.690332000	2.629990000	-0.000202000
	8	-1.379720000	1.591742000	-0.208310000
	6	-1.354654000	3.988959000	-0.044988000
	1	-2.422839000	3.893152000	-0.240784000
	1	-1.195465000	4.504244000	0.906581000
	1	-0.888163000	4.594382000	-0.827660000
	1	1.740878000	-0.105909000	2.208645000
	1	4.092116000	-0.870189000	2.190434000
	6	-2.967517000	-2.594778000	-0.168216000
	1	-2.083143000	-3.089891000	-0.568434000
	1	-3.177118000	-2.973188000	0.840997000

	1	-3.839824000	-2.769028000	-0.810535000
	6	-3.725272000	-0.431528000	0.484500000
	1	-3.872337000	-0.746242000	1.525945000
	1	-3.429171000	0.615592000	0.447842000
	1	-4.659466000	-0.575790000	-0.072613000
	7	0.170409000	-2.311020000	-0.117869000
	1	0.211942000	-2.604610000	0.866525000
	1	1.153808000	-2.345480000	-0.405461000
TS-2-NH ₂ (O2)	6	-0.598058000	-1.190718000	-0.043060000
	6	-1.206083000	-1.590546000	1.168063000
	6	-2.441918000	-2.250748000	1.193858000
	6	-3.102576000	-2.539999000	-0.007777000
	6	-2.516142000	-2.175170000	-1.227483000
	6	-1.280233000	-1.515465000	-1.237131000
	1	0.833185000	-1.563753000	-0.093710000
	1	-4.061726000	-3.053258000	0.005727000
	1	-3.019412000	-2.408525000	-2.163878000
	1	-0.837696000	-1.249881000	-2.197175000
	8	-1.553609000	1.684498000	-0.018159000
	46	0.486175000	0.761827000	-0.013364000
	8	1.896543000	-2.057594000	-0.112621000
	6	2.786310000	-1.130210000	0.005668000
	8	2.505726000	0.097133000	0.091349000
	6	4.227884000	-1.570902000	0.044405000
	1	4.892507000	-0.709971000	0.109624000
	1	4.380740000	-2.225240000	0.907511000
	1	4.453943000	-2.152005000	-0.853811000
	1	-0.703481000	-1.386946000	2.113854000
	1	-2.886673000	-2.543181000	2.143225000
	6	-1.834252000	2.590969000	-1.102996000
	1	-1.525178000	2.092913000	-2.021889000
	1	-2.910950000	2.792302000	-1.131976000
	1	-1.275048000	3.524093000	-0.982960000
	6	-2.032217000	2.178438000	1.246286000
	1	-3.110128000	2.364309000	1.179833000
	1	-1.837170000	1.402570000	1.986706000
	1	-1.515721000	3.104347000	1.525887000
	7	1.262721000	2.660152000	-0.099439000
	1	2.248854000	2.549331000	0.162232000
	1	0.865305000	3.171582000	0.698057000
INT-2-NH ₂ (O1)	6	-1.463296000	-0.596529000	0.099218000
	6	-2.228120000	-0.932396000	-1.037034000
	6	-3.631949000	-0.881819000	-1.011471000
	6	-4.302789000	-0.509201000	0.158354000

	6	-3.559533000	-0.183745000	1.301120000
	6	-2.158639000	-0.225986000	1.270482000
	1	-1.276872000	1.387675000	-0.835720000
	1	-5.389452000	-0.473198000	0.181295000
	1	-4.069845000	0.104575000	2.218232000
	1	-1.606924000	0.038402000	2.170541000
	8	2.907894000	-0.653865000	0.218051000
	46	0.560395000	-0.564973000	0.078970000
	8	-1.072066000	2.353133000	-0.892450000
	6	0.077092000	2.582690000	-0.254277000
	8	0.765888000	1.683584000	0.236966000
	6	0.445008000	4.037277000	-0.185521000
	1	-0.291977000	4.566698000	0.426083000
	1	1.436098000	4.151277000	0.251155000
	1	0.418531000	4.475908000	-1.186486000
	1	-1.731542000	-1.234392000	-1.957158000
	1	-4.196154000	-1.135852000	-1.906775000
	6	3.688475000	0.422668000	0.749377000
	1	3.076254000	0.932001000	1.493498000
	1	4.597466000	0.029245000	1.221843000
	1	3.966935000	1.131579000	-0.040998000
	6	3.619750000	-1.419833000	-0.764024000
	1	4.524922000	-1.852971000	-0.319314000
	1	2.943066000	-2.211105000	-1.087410000
	1	3.901723000	-0.787771000	-1.616684000
	7	0.547587000	-2.583580000	-0.208410000
	1	-0.413150000	-2.903475000	-0.362937000
	1	0.769931000	-2.966351000	0.719189000
INT-2-NH ₂ (O ₂)	6	-0.428853000	1.128363000	-0.021347000
	6	-0.283945000	2.002226000	1.076888000
	6	-0.843953000	3.289837000	1.076113000
	6	-1.565027000	3.741105000	-0.036382000
	6	-1.726654000	2.892887000	-1.140044000
	6	-1.170808000	1.604767000	-1.124156000
	1	-1.854040000	-0.056608000	0.865670000
	1	-1.997366000	4.739267000	-0.042807000
	1	-2.286834000	3.232428000	-2.009667000
	1	-1.322025000	0.962855000	-1.992444000
	8	2.469485000	0.422835000	0.241000000
	46	0.571605000	-0.716327000	-0.106285000
	8	-2.602353000	-0.710294000	0.945154000
	6	-2.317747000	-1.761211000	0.187653000
	8	-1.226282000	-1.912118000	-0.382442000
	6	-3.434605000	-2.756179000	0.065442000

	1	-3.078998000	-3.660128000	-0.426760000
	1	-3.834180000	-2.991199000	1.055025000
	1	-4.244243000	-2.311603000	-0.521716000
	1	0.281447000	1.681713000	1.951729000
	1	-0.715482000	3.938312000	1.941164000
	6	2.954138000	1.095120000	-0.938452000
	1	2.113603000	1.648510000	-1.356206000
	1	3.755318000	1.788250000	-0.657405000
	1	3.328907000	0.369181000	-1.668955000
	6	3.526973000	-0.264882000	0.936345000
	1	4.320696000	0.450590000	1.179702000
	1	3.098220000	-0.665082000	1.855708000
	1	3.926051000	-1.078788000	0.323360000
	7	1.677968000	-2.481337000	-0.364435000
	1	0.988861000	-3.226641000	-0.515946000
	1	2.096518000	-2.736228000	0.537666000
TS-2-CH ₃ (O1)	6	-1.610704000	0.205556000	-0.060119000
	6	-2.421707000	-0.061290000	-1.191481000
	6	-3.783082000	-0.353381000	-1.069830000
	6	-4.377067000	-0.393425000	0.200208000
	6	-3.607963000	-0.123090000	1.340777000
	6	-2.248728000	0.176971000	1.206278000
	1	-0.845163000	1.337606000	-0.233356000
	1	-5.435359000	-0.624652000	0.299361000
	1	-4.069999000	-0.141931000	2.325529000
	1	-1.671308000	0.408226000	2.099769000
	8	2.528491000	-1.471021000	0.047754000
	46	0.445844000	-0.519771000	-0.032147000
	8	-0.370056000	2.521966000	-0.335721000
	6	0.889238000	2.506725000	-0.051382000
	8	1.535777000	1.453788000	0.192140000
	6	1.584312000	3.852119000	-0.005958000
	1	2.662862000	3.727926000	0.097467000
	1	1.356546000	4.421130000	-0.911264000
	1	1.201928000	4.423948000	0.845651000
	1	-1.977522000	-0.026755000	-2.184587000
	1	-4.382703000	-0.549128000	-1.956249000
	6	3.204255000	-1.301356000	1.306880000
	1	2.519532000	-1.641747000	2.084879000
	1	4.114077000	-1.913092000	1.322193000
	1	3.459714000	-0.248483000	1.469706000
	6	3.369293000	-1.128839000	-1.068613000
	1	4.277298000	-1.743212000	-1.048797000
	1	2.800154000	-1.343172000	-1.974156000

	1	3.636485000	-0.066710000	-1.039536000
	6	-0.373357000	-2.383564000	-0.271965000
	1	0.437386000	-3.065791000	0.008564000
	1	-1.252247000	-2.544574000	0.357022000
	1	-0.641134000	-2.516565000	-1.325609000
TS-2-CH₃(O2)	6	-0.724393000	-1.043419000	0.051260000
	6	-1.525732000	-1.254105000	1.197845000
	6	-2.770069000	-1.900389000	1.141144000
	6	-3.256237000	-2.373377000	-0.085042000
	6	-2.484440000	-2.200590000	-1.242106000
	6	-1.242581000	-1.553166000	-1.162996000
	1	0.787221000	-1.583653000	0.306449000
	1	-4.218971000	-2.877938000	-0.136744000
	1	-2.848157000	-2.573392000	-2.198480000
	1	-0.661555000	-1.443704000	-2.080139000
	8	-1.226230000	2.114399000	-0.006036000
	46	0.598310000	0.807434000	-0.080270000
	8	1.727453000	-2.124568000	0.427297000
	6	2.708249000	-1.323609000	0.120317000
	8	2.545724000	-0.115031000	-0.170681000
	6	4.083413000	-1.936183000	0.124283000
	1	4.270116000	-2.412116000	1.090741000
	1	4.131541000	-2.715917000	-0.641671000
	1	4.839969000	-1.177516000	-0.073056000
	1	-1.170897000	-0.909802000	2.170488000
	1	-3.356458000	-2.039981000	2.048152000
	6	-2.247245000	1.902405000	-0.998791000
	1	-1.740041000	1.770125000	-1.954558000
	1	-2.836648000	1.009854000	-0.765563000
	1	-2.897254000	2.784175000	-1.040707000
	6	-1.779063000	2.385343000	1.294400000
	1	-2.335656000	1.518247000	1.666348000
	1	-0.942921000	2.604253000	1.959092000
	1	-2.442324000	3.256048000	1.233301000
	6	1.608705000	2.612749000	-0.270316000
	1	1.302999000	3.062803000	-1.222484000
	1	1.309916000	3.260960000	0.561778000
	1	2.687661000	2.433215000	-0.255128000
INT-2-CH₃(O1)	6	-1.509035000	-0.541035000	0.009379000
	6	-2.264640000	-0.483968000	-1.183361000
	6	-3.659240000	-0.322015000	-1.165734000
	6	-4.343277000	-0.222826000	0.051704000
	6	-3.617915000	-0.284350000	1.248655000
	6	-2.224312000	-0.443552000	1.224792000

	1	-1.234258000	1.592229000	-0.173328000
	1	-5.423920000	-0.100792000	0.068217000
	1	-4.135980000	-0.209552000	2.203154000
	1	-1.690085000	-0.488971000	2.171977000
	8	2.842242000	-0.930721000	-0.008319000
	46	0.522949000	-0.673983000	-0.004339000
	8	-0.963193000	2.544193000	-0.170863000
	6	0.362126000	2.611463000	-0.011283000
	8	1.076078000	1.612498000	0.092265000
	6	0.882907000	4.021183000	0.033971000
	1	0.469662000	4.532547000	0.908627000
	1	1.970590000	4.015930000	0.089862000
	1	0.552678000	4.568400000	-0.853147000
	1	-1.763194000	-0.563906000	-2.146000000
	1	-4.208593000	-0.276246000	-2.104400000
	6	3.509239000	-0.581746000	1.213626000
	1	2.951384000	-1.046649000	2.028040000
	1	4.535917000	-0.968433000	1.203237000
	1	3.527127000	0.506111000	1.351433000
	6	3.525739000	-0.420243000	-1.162214000
	1	4.557006000	-0.794019000	-1.182554000
	1	2.988551000	-0.782081000	-2.040427000
	1	3.531211000	0.676294000	-1.157715000
	6	0.198884000	-2.708900000	-0.107782000
	1	-0.328383000	-2.986249000	-1.026328000
	1	1.206889000	-3.142486000	-0.109138000
	1	-0.366138000	-3.080718000	0.752910000
INT-2-CH ₃ (O ₂)	6	0.825329000	0.983525000	0.047515000
	6	1.712233000	1.163580000	1.133899000
	6	2.812399000	2.032896000	1.073730000
	6	3.066677000	2.760847000	-0.096556000
	6	2.206879000	2.614942000	-1.193130000
	6	1.106446000	1.747342000	-1.109641000
	1	-0.796087000	1.614020000	0.657626000
	1	3.919158000	3.434893000	-0.151324000
	1	2.390684000	3.178750000	-2.106705000
	1	0.448923000	1.668854000	-1.977351000
	8	1.335732000	-2.021324000	0.218476000
	46	-0.491456000	-0.779192000	-0.117522000
	8	-1.697549000	2.075470000	0.811579000
	6	-2.617374000	1.370523000	0.184376000
	8	-2.380941000	0.272632000	-0.353718000
	6	-3.984456000	1.992671000	0.156762000
	1	-4.701700000	1.308276000	-0.294080000

	1	-4.292946000	2.247903000	1.174121000
	1	-3.945042000	2.922320000	-0.418804000
	1	1.547544000	0.609123000	2.058875000
	1	3.469719000	2.142922000	1.935209000
	6	2.105754000	-2.342990000	-0.953689000
	1	2.190577000	-1.427832000	-1.539827000
	1	3.102915000	-2.684553000	-0.653019000
	1	1.608824000	-3.123278000	-1.542201000
	6	1.264849000	-3.119517000	1.145147000
	1	2.280457000	-3.412664000	1.435103000
	1	0.717951000	-2.766049000	2.019226000
	1	0.744753000	-3.975428000	0.701643000
	6	-1.615463000	-2.535982000	-0.388906000
	1	-2.564213000	-2.278527000	-0.872676000
	1	-1.058276000	-3.243265000	-1.016813000
	1	-1.813845000	-2.993861000	0.589250000
TS-2-Ph(O1)	6	-0.345991000	1.708419000	-0.076983000
	6	-0.173257000	2.387315000	1.156528000
	6	0.603305000	3.544870000	1.257059000
	6	1.227184000	4.065733000	0.114254000
	6	1.065470000	3.428815000	-1.124148000
	6	0.295499000	2.265879000	-1.211264000
	1	-1.666909000	1.443865000	-0.324724000
	1	1.829864000	4.968324000	0.187191000
	1	1.541966000	3.837615000	-2.012471000
	1	0.174644000	1.786253000	-2.180561000
	8	-0.508917000	-2.749457000	0.384516000
	46	-0.469764000	-0.465257000	0.110748000
	8	-2.938162000	1.448788000	-0.507797000
	6	-3.416187000	0.308420000	-0.142382000
	8	-2.700307000	-0.661111000	0.227860000
	6	-4.924374000	0.170572000	-0.149951000
	1	-5.217030000	-0.876091000	-0.059019000
	1	-5.334087000	0.730957000	0.697007000
	1	-5.339725000	0.603085000	-1.063397000
	1	-0.673060000	2.010364000	2.047295000
	1	0.718619000	4.045828000	2.215780000
	6	1.534367000	-0.448507000	-0.054913000
	6	2.112604000	-0.876568000	-1.260923000
	6	2.369574000	-0.165962000	1.036787000
	6	3.501994000	-1.044683000	-1.366160000
	1	1.487956000	-1.085242000	-2.127855000
	6	3.758917000	-0.337417000	0.932284000
	1	1.948731000	0.186669000	1.975707000

	6	4.329980000	-0.777304000	-0.268431000
	1	3.934069000	-1.381186000	-2.306794000
	1	4.393119000	-0.120962000	1.790030000
	1	5.407083000	-0.904110000	-0.349803000
	6	-1.044590000	-3.485223000	-0.727938000
	1	-1.883143000	-2.908509000	-1.118274000
	1	-0.284054000	-3.620825000	-1.506923000
	1	-1.398020000	-4.465739000	-0.386962000
	6	0.554377000	-3.456314000	1.042954000
	1	1.403366000	-3.604039000	0.365850000
	1	0.866883000	-2.850920000	1.893572000
	1	0.184715000	-4.427563000	1.392704000
TS-2-Ph(O2)	6	2.100607000	0.260274000	0.008624000
	6	2.753742000	-0.161484000	1.189856000
	6	4.017837000	-0.768492000	1.172256000
	6	4.682678000	-0.960592000	-0.046646000
	6	4.075990000	-0.537115000	-1.236738000
	6	2.809995000	0.064469000	-1.198790000
	1	1.591843000	1.727109000	0.092313000
	1	5.665368000	-1.427216000	-0.067721000
	1	4.589798000	-0.673213000	-2.186912000
	1	2.365600000	0.391896000	-2.139683000
	8	0.037655000	-2.148750000	0.106684000
	46	-0.174201000	0.084264000	-0.031274000
	8	1.425601000	2.837802000	0.117550000
	6	0.158917000	3.071788000	-0.037629000
	8	-0.706880000	2.166447000	-0.140174000
	6	-0.248548000	4.520832000	-0.105165000
	1	0.172410000	5.063716000	0.744902000
	1	0.164607000	4.963288000	-1.016903000
	1	-1.334124000	4.613421000	-0.113982000
	1	2.267575000	-0.011390000	2.154687000
	1	4.486751000	-1.084643000	2.102601000
	6	-2.187519000	-0.275665000	-0.073916000
	6	-2.725047000	-1.215586000	-0.966228000
	6	-3.052383000	0.407144000	0.794666000
	6	-4.106254000	-1.466569000	-0.993144000
	1	-2.074704000	-1.766246000	-1.643304000
	6	-4.431781000	0.145839000	0.780867000
	1	-2.662040000	1.154738000	1.482541000
	6	-4.963244000	-0.789797000	-0.115899000
	1	-4.509136000	-2.194125000	-1.695573000
	1	-5.088984000	0.678699000	1.465858000
	1	-6.032650000	-0.987914000	-0.132164000

	6	0.984576000	-2.846063000	-0.723688000
	1	0.928555000	-2.402500000	-1.717263000
	1	2.000359000	-2.742363000	-0.329315000
	1	0.704630000	-3.904811000	-0.771847000
	6	-0.044084000	-2.711072000	1.429133000
	1	0.904821000	-2.585366000	1.963054000
	1	-0.841624000	-2.183809000	1.952675000
	1	-0.289695000	-3.776881000	1.356824000
INT-2-Ph(O1)	6	-0.783133000	1.349927000	0.115575000
	6	-1.251593000	1.858833000	1.346734000
	6	-1.905169000	3.096704000	1.425091000
	6	-2.106949000	3.864789000	0.270443000
	6	-1.643614000	3.383707000	-0.958952000
	6	-0.983726000	2.145489000	-1.031418000
	1	-2.653999000	0.422156000	-0.610526000
	1	-2.615183000	4.824440000	0.330132000
	1	-1.790229000	3.969805000	-1.864284000
	1	-0.623607000	1.804569000	-2.000313000
	8	0.867731000	-2.707668000	-0.028212000
	46	-0.003361000	-0.530519000	0.030028000
	8	-3.454725000	-0.154166000	-0.675622000
	6	-3.144520000	-1.376480000	-0.232443000
	8	-2.011544000	-1.691032000	0.136812000
	6	-4.314270000	-2.320361000	-0.229564000
	1	-4.749473000	-2.371673000	-1.231506000
	1	-3.993616000	-3.310513000	0.091152000
	1	-5.087188000	-1.941530000	0.445652000
	1	-1.112089000	1.284559000	2.260658000
	1	-2.257080000	3.460496000	2.388768000
	6	1.796133000	0.399039000	-0.034159000
	6	2.360013000	0.843856000	-1.244294000
	6	2.584939000	0.487611000	1.129170000
	6	3.673413000	1.335060000	-1.297741000
	1	1.777417000	0.813147000	-2.163336000
	6	3.898054000	0.981519000	1.081316000
	1	2.181485000	0.171488000	2.089614000
	6	4.449774000	1.406024000	-0.133950000
	1	4.086856000	1.666896000	-2.248735000
	1	4.486726000	1.037197000	1.995538000
	1	5.466326000	1.791284000	-0.172544000
	6	1.893432000	-3.010225000	-0.984849000
	1	1.599396000	-2.547002000	-1.927446000
	1	2.860476000	-2.605235000	-0.664137000
	1	1.972548000	-4.096620000	-1.115133000

	6	1.122119000	-3.307485000	1.249942000
	1	2.037071000	-2.899058000	1.696871000
	1	0.266580000	-3.080967000	1.887754000
	1	1.221084000	-4.394670000	1.141272000
INT-2-Ph(O2)	6	2.016292000	-0.055029000	-0.003617000
	6	2.717379000	-0.307611000	1.198145000
	6	4.076171000	-0.659540000	1.216184000
	6	4.788626000	-0.762067000	0.014241000
	6	4.131410000	-0.503593000	-1.195938000
	6	2.772399000	-0.154195000	-1.194403000
	1	1.824622000	1.800493000	0.067102000
	1	5.842172000	-1.033531000	0.020913000
	1	4.676417000	-0.572053000	-2.136194000
	1	2.292102000	0.043882000	-2.153899000
	8	-0.150233000	-2.259228000	0.055980000
	46	-0.163465000	-0.022218000	-0.040655000
	8	1.687182000	2.803250000	0.060566000
	6	0.394448000	3.037846000	-0.061809000
	8	-0.460515000	2.137981000	-0.122875000
	6	0.025265000	4.492567000	-0.129507000
	1	0.440220000	5.019328000	0.733936000
	1	0.466721000	4.933351000	-1.028405000
	1	-1.057547000	4.604742000	-0.156649000
	1	2.195217000	-0.228153000	2.152843000
	1	4.578258000	-0.849471000	2.163628000
	6	-2.242277000	-0.160923000	-0.063230000
	6	-2.895873000	-1.131647000	-0.843754000
	6	-3.040434000	0.698655000	0.713251000
	6	-4.296059000	-1.239154000	-0.854855000
	1	-2.313749000	-1.825223000	-1.448889000
	6	-4.440210000	0.588166000	0.720807000
	1	-2.574929000	1.475211000	1.318689000
	6	-5.074543000	-0.380973000	-0.067400000
	1	-4.776736000	-1.995229000	-1.473981000
	1	-5.033858000	1.261497000	1.337473000
	1	-6.159246000	-0.465324000	-0.068770000
	6	0.762846000	-3.013936000	-0.762293000
	1	0.740863000	-2.574106000	-1.759080000
	1	1.779627000	-2.965709000	-0.359879000
	1	0.423477000	-4.055256000	-0.806665000
	6	-0.275754000	-2.810821000	1.379974000
	1	0.671840000	-2.729833000	1.924897000
	1	-1.052746000	-2.241545000	1.890055000
	1	-0.572935000	-3.863522000	1.308860000

TS-2-CN(O1)	6	-1.535360000	0.405442000	0.038705000
	6	-2.182876000	0.365652000	-1.226466000
	6	-3.556088000	0.147174000	-1.328293000
	6	-4.316028000	-0.050095000	-0.165439000
	6	-3.705596000	-0.024539000	1.097386000
	6	-2.330948000	0.186735000	1.196013000
	1	-0.835343000	1.504516000	0.167673000
	1	-5.387034000	-0.221022000	-0.243669000
	1	-4.302147000	-0.174450000	1.993520000
	1	-1.862204000	0.212759000	2.176726000
	8	2.445671000	-1.460184000	-0.051704000
	46	0.441562000	-0.443592000	0.028455000
	8	-0.225643000	2.697794000	0.250951000
	6	1.024859000	2.516533000	0.065965000
	8	1.557658000	1.372758000	-0.092070000
	6	1.912842000	3.741077000	0.016058000
	1	1.708508000	4.285900000	-0.911117000
	1	1.673747000	4.405750000	0.849531000
	1	2.965841000	3.460693000	0.044687000
	1	-1.600968000	0.537175000	-2.129137000
	1	-4.037433000	0.130847000	-2.302745000
	6	3.305179000	-1.190176000	1.074147000
	1	2.722689000	-1.388638000	1.974283000
	1	4.169700000	-1.861901000	1.037190000
	1	3.637796000	-0.146909000	1.063401000
	6	3.130755000	-1.315771000	-1.312426000
	1	3.998836000	-1.983643000	-1.329965000
	1	2.426303000	-1.606569000	-2.092311000
	1	3.450559000	-0.278859000	-1.460466000
	6	-0.486348000	-2.199450000	0.141368000
	7	-0.974933000	-3.264122000	0.201994000
TS-2-CN(O2)	6	-0.907666000	-1.106563000	-0.028666000
	6	-1.564610000	-1.311275000	1.205403000
	6	-2.931542000	-1.603374000	1.259008000
	6	-3.669218000	-1.701036000	0.070890000
	6	-3.037537000	-1.515064000	-1.166928000
	6	-1.671395000	-1.219254000	-1.212029000
	1	0.275171000	-1.815091000	-0.122492000
	1	-4.731771000	-1.929687000	0.109026000
	1	-3.608298000	-1.604320000	-2.088404000
	1	-1.188981000	-1.088051000	-2.179390000
	8	-1.167370000	1.841195000	-0.046547000
	46	0.580054000	0.520512000	0.001228000
	8	1.243659000	-2.591466000	-0.181237000

	6	2.309297000	-1.899805000	-0.033096000
	8	2.325235000	-0.635100000	0.089112000
	6	3.626508000	-2.637385000	-0.002712000
	1	4.453850000	-1.947426000	0.158284000
	1	3.600110000	-3.386724000	0.792875000
	1	3.760067000	-3.165034000	-0.951273000
	1	-0.998214000	-1.254165000	2.133661000
	1	-3.420037000	-1.759808000	2.218051000
	6	-1.321166000	2.653868000	-1.232426000
	1	-1.162987000	2.000560000	-2.090057000
	1	-2.339017000	3.056284000	-1.253113000
	1	-0.590246000	3.468356000	-1.237707000
	6	-1.432547000	2.583162000	1.165133000
	1	-2.442138000	3.002701000	1.106325000
	1	-1.373719000	1.876709000	1.992678000
	1	-0.696103000	3.382227000	1.294957000
	6	1.798949000	2.166933000	0.060563000
	7	2.481888000	3.120237000	0.094085000
INT-2-CN(O1)	6	-1.465933000	-0.508259000	0.012472000
	6	-2.180312000	-0.379539000	-1.191241000
	6	-3.573909000	-0.201814000	-1.172719000
	6	-4.264294000	-0.168150000	0.043530000
	6	-3.556947000	-0.314668000	1.243850000
	6	-2.165841000	-0.490870000	1.231113000
	1	-1.439061000	1.704184000	-0.287380000
	1	-5.342958000	-0.033780000	0.056936000
	1	-4.086068000	-0.295514000	2.194027000
	1	-1.634944000	-0.609065000	2.172218000
	8	2.855856000	-0.648962000	-0.064373000
	46	0.547794000	-0.568233000	-0.008320000
	8	-1.138062000	2.640627000	-0.208287000
	6	0.174375000	2.663394000	0.015972000
	8	0.868720000	1.643636000	0.088345000
	6	0.732051000	4.047246000	0.180374000
	1	0.304804000	4.501525000	1.079566000
	1	1.816452000	4.004722000	0.268838000
	1	0.443438000	4.668444000	-0.671417000
	1	-1.661688000	-0.412748000	-2.146219000
	1	-4.112437000	-0.093396000	-2.111476000
	6	3.531994000	-0.420053000	1.182573000
	1	3.016592000	-1.011371000	1.940608000
	1	4.574403000	-0.750615000	1.105429000
	1	3.500636000	0.642187000	1.453348000
	6	3.492871000	0.019977000	-1.164978000

	1	4.530712000	-0.321616000	-1.254314000
	1	2.940680000	-0.249074000	-2.066607000
	1	3.470240000	1.106939000	-1.025294000
	6	0.311542000	-2.545253000	-0.067531000
	7	0.224998000	-3.715226000	-0.104501000
INT-2-CN(O2)	6	1.016290000	-0.811091000	-0.100300000
	6	1.336888000	-1.659990000	0.970730000
	6	2.536059000	-2.391075000	0.963267000
	6	3.415699000	-2.288135000	-0.120412000
	6	3.097564000	-1.446333000	-1.194074000
	6	1.906849000	-0.705023000	-1.181086000
	1	1.529402000	0.987741000	1.251857000
	1	4.341651000	-2.858091000	-0.128822000
	1	3.776064000	-1.360950000	-2.040351000
	1	1.682672000	-0.045911000	-2.017903000
	8	-1.763800000	-1.723058000	0.164789000
	46	-0.745956000	0.220244000	-0.130406000
	8	1.837166000	1.924544000	1.247235000
	6	1.235373000	2.573547000	0.255405000
	8	0.339246000	2.077599000	-0.442522000
	6	1.745349000	3.966954000	0.039332000
	1	1.096598000	4.498111000	-0.655120000
	1	1.800489000	4.495370000	0.994031000
	1	2.759029000	3.912817000	-0.369990000
	1	0.658589000	-1.766797000	1.815165000
	1	2.775650000	-3.041284000	1.802027000
	6	-2.337056000	-2.287629000	-1.034751000
	1	-1.561152000	-2.264616000	-1.799952000
	1	-2.633753000	-3.323032000	-0.836087000
	1	-3.204709000	-1.702986000	-1.357838000
	6	-2.667725000	-1.800801000	1.288598000
	1	-2.934281000	-2.849629000	1.457433000
	1	-2.135378000	-1.409376000	2.155672000
	1	-3.566016000	-1.204506000	1.101778000
	6	-2.610317000	1.276987000	-0.176479000
	7	-3.631663000	1.857825000	-0.198658000
TS-2-F(O1)	6	-1.569732000	0.214372000	-0.075090000
	6	-2.268064000	-0.198978000	-1.237523000
	6	-3.593202000	-0.628834000	-1.165116000
	6	-4.242060000	-0.678319000	0.077918000
	6	-3.571987000	-0.285179000	1.245536000
	6	-2.249195000	0.154278000	1.168320000
	1	-1.006081000	1.400422000	-0.252850000
	1	-5.273149000	-1.019147000	0.135640000

	1	-4.082980000	-0.318421000	2.204564000
	1	-1.740983000	0.480078000	2.073311000
	8	2.573466000	-1.175145000	0.242693000
	46	0.473835000	-0.376781000	0.030185000
	8	-0.546182000	2.630324000	-0.346937000
	6	0.683532000	2.593952000	-0.008591000
	8	1.313417000	1.519691000	0.256485000
	6	1.436669000	3.902400000	0.072317000
	1	2.431079000	3.754678000	0.492900000
	1	1.524083000	4.320425000	-0.935190000
	1	0.870509000	4.614025000	0.678104000
	1	-1.771185000	-0.158734000	-2.204033000
	1	-4.122014000	-0.927121000	-2.067016000
	6	3.649631000	-0.526520000	-0.458720000
	1	3.446186000	0.543065000	-0.439579000
	1	4.596169000	-0.735748000	0.052939000
	1	3.703486000	-0.884723000	-1.493813000
	6	2.753331000	-2.602159000	0.321212000
	1	3.656862000	-2.817079000	0.903211000
	1	1.870129000	-3.009619000	0.808743000
	1	2.845950000	-3.032287000	-0.682674000
	9	-0.182626000	-2.260769000	-0.169139000
TS-2-F(O2)	6	0.502056000	-1.206120000	-0.025320000
	6	1.195155000	-1.522229000	-1.218057000
	6	2.420843000	-2.191778000	-1.184445000
	6	2.980111000	-2.557698000	0.048547000
	6	2.308269000	-2.266359000	1.244463000
	6	1.081430000	-1.598658000	1.204886000
	1	-0.787160000	-1.541411000	-0.107420000
	1	3.935008000	-3.077323000	0.077018000
	1	2.738828000	-2.564103000	2.197519000
	1	0.556980000	-1.390849000	2.135625000
	8	1.608687000	1.543600000	-0.048845000
	46	-0.420631000	0.747070000	0.020786000
	8	-1.993780000	-2.018441000	-0.166788000
	6	-2.794584000	-1.033697000	-0.028834000
	8	-2.420050000	0.175008000	0.097983000
	6	-4.278633000	-1.322322000	-0.028402000
	1	-4.494456000	-2.125624000	0.680099000
	1	-4.848779000	-0.429193000	0.225114000
	1	-4.567549000	-1.670758000	-1.024646000
	1	0.760398000	-1.252677000	-2.178735000
	1	2.938475000	-2.432642000	-2.109857000
	6	1.938011000	2.278618000	1.153480000

	1	1.815996000	1.589157000	1.989100000
	1	2.981038000	2.606518000	1.092141000
	1	1.269210000	3.136581000	1.265002000
	6	1.839153000	2.332807000	-1.239620000
	1	2.883647000	2.661295000	-1.248493000
	1	1.648800000	1.682335000	-2.093519000
	1	1.164015000	3.192815000	-1.257383000
	9	-1.039461000	2.685994000	0.087031000
INT-2-F(O1)	6	-1.492778000	-0.497481000	0.129858000
	6	-2.211154000	-1.273991000	-0.791704000
	6	-3.614138000	-1.253636000	-0.781920000
	6	-4.305090000	-0.475586000	0.155331000
	6	-3.587409000	0.287236000	1.084307000
	6	-2.184283000	0.281461000	1.071576000
	1	-0.763704000	1.251067000	-1.392624000
	1	-5.392389000	-0.466577000	0.164134000
	1	-4.114514000	0.890400000	1.820637000
	1	-1.643753000	0.883368000	1.798250000
	8	2.828116000	-0.651661000	0.247132000
	46	0.504480000	-0.521187000	0.137110000
	8	-0.564790000	2.216909000	-1.394269000
	6	0.201069000	2.495800000	-0.344116000
	8	0.632437000	1.626597000	0.428489000
	6	0.488907000	3.955932000	-0.168073000
	1	-0.435617000	4.467749000	0.116866000
	1	1.240543000	4.097851000	0.606702000
	1	0.826792000	4.385594000	-1.114262000
	1	-1.682510000	-1.902974000	-1.501840000
	1	-4.164405000	-1.854087000	-1.503401000
	6	3.699344000	0.474614000	0.404579000
	1	3.126693000	1.262108000	0.894556000
	1	4.559487000	0.199642000	1.027335000
	1	4.056067000	0.828694000	-0.571408000
	6	3.479421000	-1.778434000	-0.361859000
	1	4.312287000	-2.112321000	0.269354000
	1	2.726017000	-2.561325000	-0.446206000
	1	3.860210000	-1.509010000	-1.355574000
	9	0.474807000	-2.523982000	-0.195366000
INT-2-F(O2)	6	-0.400917000	1.082300000	-0.047749000
	6	-0.347727000	1.905934000	1.089947000
	6	-1.008791000	3.145084000	1.102600000
	6	-1.719802000	3.575364000	-0.023449000
	6	-1.774822000	2.759698000	-1.161393000
	6	-1.124489000	1.517268000	-1.172248000

	1	-1.941628000	-0.100166000	1.008560000
	1	-2.228099000	4.536492000	-0.014768000
	1	-2.326637000	3.086326000	-2.040328000
	1	-1.187337000	0.891482000	-2.060662000
	8	2.471264000	0.495366000	0.208618000
	46	0.603519000	-0.656953000	-0.101466000
	8	-2.653312000	-0.784343000	1.001911000
	6	-2.311133000	-1.756196000	0.160492000
	8	-1.215696000	-1.808822000	-0.414618000
	6	-3.380923000	-2.788169000	-0.042557000
	1	-2.986952000	-3.626611000	-0.614446000
	1	-3.757221000	-3.127991000	0.925499000
	1	-4.217107000	-2.332559000	-0.582069000
	1	0.212341000	1.593384000	1.969247000
	1	-0.962119000	3.770599000	1.991512000
	6	3.051871000	1.017265000	-1.005115000
	1	2.267221000	1.569388000	-1.522221000
	1	3.875741000	1.692526000	-0.748972000
	1	3.420647000	0.202190000	-1.637517000
	6	3.449440000	-0.189333000	1.024245000
	1	4.286790000	0.490734000	1.215011000
	1	2.957065000	-0.444502000	1.962752000
	1	3.788687000	-1.100535000	0.525800000
	9	1.735828000	-2.412645000	-0.180656000

Table S3. Cartesian coordinates of the optimized stationary points involved in the discussion on the effects of the six neutral ligands on C–H activation, calculated at the B3LYP/DGDZVP level of theory in CH₂Cl₂ solvent.

Names	Cartesian Coordinates			
TS-2-NMe ₃ (O1)	6	-1.494377000	0.948148000	0.030438000
	6	-2.429126000	0.500097000	-0.932644000
	6	-3.796425000	0.456790000	-0.648288000
	6	-4.258782000	0.843657000	0.617929000
	6	-3.354085000	1.288122000	1.592576000
	6	-1.989116000	1.342135000	1.297085000
	1	-0.670281000	1.887722000	-0.505155000
	1	-5.322267000	0.804678000	0.842553000
	1	-3.715099000	1.596349000	2.571073000
	1	-1.297933000	1.712336000	2.052215000
	46	0.439561000	-0.045500000	0.141837000
	8	-0.027115000	2.912255000	-0.916316000
	6	1.184742000	2.767445000	-0.531317000

	8	1.624564000	1.708604000	0.014736000
	6	2.135875000	3.920015000	-0.753923000
	1	1.679673000	4.848994000	-0.404005000
	1	3.083255000	3.746411000	-0.243769000
	1	2.316438000	4.023236000	-1.828503000
	1	-2.077853000	0.191841000	-1.914109000
	1	-4.501092000	0.120550000	-1.405490000
	6	-0.933229000	-2.497423000	-0.673537000
	8	-0.551454000	-2.247705000	-1.830265000
	8	-0.657886000	-1.787764000	0.384631000
	6	-1.807393000	-3.711593000	-0.373624000
	1	-1.433794000	-4.251292000	0.501017000
	1	-2.823434000	-3.375074000	-0.141566000
	1	-1.842712000	-4.379304000	-1.236455000
	7	2.376631000	-1.128727000	0.419034000
	6	2.207634000	-2.594350000	0.572137000
	1	1.541174000	-2.803804000	1.409101000
	1	1.774183000	-3.009289000	-0.338156000
	1	3.183219000	-3.066559000	0.754270000
	6	3.240392000	-0.856497000	-0.758640000
	1	2.760181000	-1.247656000	-1.657751000
	1	3.383393000	0.218980000	-0.865722000
	1	4.219218000	-1.341593000	-0.635152000
	6	3.008554000	-0.579010000	1.645922000
	1	3.134409000	0.498906000	1.541613000
	1	2.369339000	-0.785906000	2.507149000
	1	3.990916000	-1.043788000	1.812142000
TS-2-NMe ₃ (O ₂)	6	1.737897000	0.510306000	0.076905000
	6	2.325277000	0.286835000	1.347547000
	6	3.687342000	0.005544000	1.482560000
	6	4.498921000	-0.066567000	0.341223000
	6	3.949863000	0.158114000	-0.929411000
	6	2.588108000	0.445369000	-1.055331000
	1	1.155364000	1.719386000	0.124922000
	1	5.559421000	-0.284945000	0.442800000
	1	4.584282000	0.116482000	-1.811674000
	1	2.178107000	0.645213000	-2.043632000
	46	-0.350947000	-0.064499000	-0.194796000
	8	0.775189000	2.949410000	0.168813000
	6	-0.462038000	2.949395000	-0.164683000
	8	-1.123957000	1.896491000	-0.399265000
	6	-1.157762000	4.287233000	-0.271803000
	1	-2.163887000	4.169670000	-0.673421000
	1	-1.212233000	4.736647000	0.724369000

	1	-0.571373000	4.956543000	-0.906262000
	1	1.707524000	0.361400000	2.240673000
	1	4.118420000	-0.152583000	2.468318000
	6	-3.215530000	-0.381396000	0.452140000
	8	-2.914542000	-0.017085000	1.602844000
	8	-2.369337000	-0.628547000	-0.507858000
	6	-4.675170000	-0.573977000	0.047193000
	1	-5.317926000	-0.601232000	0.929374000
	1	-4.983659000	0.262927000	-0.588903000
	1	-4.800892000	-1.490997000	-0.535147000
	7	0.115836000	-2.225062000	-0.176399000
	6	-0.464653000	-2.766513000	-1.438988000
	1	0.078369000	-2.353084000	-2.291669000
	1	-0.369746000	-3.860875000	-1.453336000
	1	-1.514852000	-2.487937000	-1.507230000
	6	-0.593721000	-2.818203000	0.992236000
	1	-1.652972000	-2.575029000	0.941212000
	1	-0.469146000	-3.909913000	0.990357000
	1	-0.174824000	-2.412747000	1.915007000
	6	1.541269000	-2.642680000	-0.112236000
	1	1.992473000	-2.292831000	0.814697000
	1	1.603358000	-3.738600000	-0.148451000
	1	2.089265000	-2.227992000	-0.956993000
INT-2-NMe ₃ (O1)	6	1.512260000	-0.533899000	-0.291430000
	6	2.082163000	-1.339312000	0.709388000
	6	3.421965000	-1.752532000	0.610481000
	6	4.198150000	-1.380368000	-0.492217000
	6	3.631647000	-0.586110000	-1.498357000
	6	2.299488000	-0.161767000	-1.396440000
	1	1.866418000	1.078811000	1.174101000
	1	5.233141000	-1.705006000	-0.569015000
	1	4.226121000	-0.292410000	-2.361216000
	1	1.881591000	0.463491000	-2.183351000
	46	-0.401541000	0.117359000	-0.223222000
	8	1.982025000	2.042062000	1.362503000
	6	1.127493000	2.733954000	0.614814000
	8	0.263592000	2.208202000	-0.099657000
	6	1.308820000	4.220798000	0.707058000
	1	2.266468000	4.492395000	0.252262000
	1	0.497951000	4.729585000	0.188235000
	1	1.343116000	4.526771000	1.755694000
	1	1.483018000	-1.656589000	1.558644000
	1	3.851672000	-2.370105000	1.396675000
	6	-1.138199000	-2.644590000	0.586143000

	8	-0.947180000	-2.303929000	1.768438000
	8	-1.034146000	-1.872058000	-0.455803000
	6	-1.516394000	-4.084085000	0.241538000
	1	-1.858699000	-4.614960000	1.132141000
	1	-2.289077000	-4.112625000	-0.531396000
	1	-0.634333000	-4.598054000	-0.156304000
	7	-2.621648000	0.811648000	-0.293277000
	6	-2.749649000	2.283312000	-0.371754000
	1	-2.216437000	2.654796000	-1.249176000
	1	-3.806854000	2.581200000	-0.441965000
	1	-2.312133000	2.740236000	0.517864000
	6	-3.324774000	0.322027000	0.914334000
	1	-4.393287000	0.586094000	0.882357000
	1	-3.225734000	-0.761678000	0.983412000
	1	-2.877515000	0.769780000	1.805168000
	6	-3.222912000	0.201248000	-1.501553000
	1	-2.714692000	0.578892000	-2.392825000
	1	-3.099151000	-0.881967000	-1.460150000
	1	-4.293856000	0.445015000	-1.575896000
INT-2-NMe ₃ (O ₂)	6	1.679592000	-0.237470000	-0.030601000
	6	2.281952000	-0.298926000	1.239604000
	6	3.680683000	-0.250401000	1.374355000
	6	4.492825000	-0.145096000	0.240599000
	6	3.900884000	-0.081973000	-1.028598000
	6	2.506030000	-0.121803000	-1.162806000
	1	1.495050000	1.842994000	0.860134000
	1	5.574758000	-0.110876000	0.342563000
	1	4.524913000	0.002820000	-1.916030000
	1	2.068562000	-0.061403000	-2.157597000
	46	-0.330380000	-0.209978000	-0.223587000
	8	1.274741000	2.798077000	0.744973000
	6	0.280793000	2.917798000	-0.133868000
	8	-0.305614000	1.954934000	-0.639732000
	6	-0.066308000	4.342372000	-0.456048000
	1	-0.874596000	4.373811000	-1.184764000
	1	-0.369267000	4.856891000	0.460492000
	1	0.816349000	4.855963000	-0.847098000
	1	1.670378000	-0.395436000	2.135853000
	1	4.127190000	-0.297286000	2.365386000
	6	-3.199119000	0.501582000	0.382838000
	8	-2.775957000	0.905327000	1.488467000
	8	-2.491166000	-0.107498000	-0.513909000
	6	-4.661746000	0.722966000	-0.005754000
	1	-5.244958000	1.078725000	0.846299000

	1	-4.714730000	1.468512000	-0.807021000
	1	-5.100829000	-0.200920000	-0.394406000
	7	-0.495150000	-2.401421000	-0.041909000
	6	-1.220412000	-2.846734000	-1.264656000
	1	-0.593135000	-2.669833000	-2.140925000
	1	-1.446327000	-3.920524000	-1.198217000
	1	-2.146735000	-2.281251000	-1.361660000
	6	-1.333981000	-2.676237000	1.157144000
	1	-2.273725000	-2.131747000	1.074184000
	1	-1.539957000	-3.753253000	1.235501000
	1	-0.805281000	-2.348616000	2.054419000
	6	0.765646000	-3.179304000	0.068634000
	1	1.302027000	-2.894236000	0.973387000
	1	0.536143000	-4.253178000	0.109531000
	1	1.400618000	-2.979573000	-0.795111000
TS-2- $\text{PMe}_3(\text{O1})$	6	1.941897000	0.584514000	-0.043085000
	6	2.679278000	0.020099000	1.021734000
	6	3.986489000	-0.445989000	0.841019000
	6	4.588355000	-0.363498000	-0.422446000
	6	3.883195000	0.197099000	-1.496229000
	6	2.578657000	0.666314000	-1.302072000
	1	1.346549000	1.836671000	0.337879000
	1	5.602865000	-0.728198000	-0.567822000
	1	4.351211000	0.270511000	-2.475772000
	1	2.051162000	1.112683000	-2.144299000
	46	-0.240864000	0.140787000	-0.131105000
	8	1.027539000	2.960555000	0.614425000
	6	-0.237322000	3.084468000	0.419870000
	8	-0.987955000	2.126643000	0.072804000
	6	-0.831768000	4.457372000	0.613412000
	1	-0.580321000	4.825435000	1.611594000
	1	-0.387577000	5.144407000	-0.112814000
	1	-1.913405000	4.432561000	0.484301000
	1	2.228238000	-0.049567000	2.010286000
	1	4.535399000	-0.872188000	1.678256000
	6	0.214626000	-2.664025000	0.563283000
	8	-0.344107000	-2.410553000	1.645904000
	8	0.360557000	-1.830088000	-0.426264000
	6	0.804982000	-4.042873000	0.280858000
	1	1.892351000	-3.961929000	0.184741000
	1	0.565931000	-4.734465000	1.090616000
	1	0.422210000	-4.434913000	-0.665993000
	15	-2.527750000	-0.490744000	-0.291024000
	6	-3.427727000	-0.286407000	1.297349000

	1	-4.490193000	-0.520579000	1.173697000
	1	-2.991018000	-0.953777000	2.043820000
	1	-3.325137000	0.745233000	1.643624000
	6	-2.893845000	-2.208782000	-0.819957000
	1	-2.520084000	-2.906773000	-0.068512000
	1	-3.973646000	-2.346679000	-0.937047000
	1	-2.397911000	-2.415277000	-1.771319000
	6	-3.450144000	0.559409000	-1.485060000
	1	-4.517798000	0.316616000	-1.470416000
	1	-3.311887000	1.610709000	-1.222596000
	1	-3.059259000	0.395820000	-2.493047000
TS-2-PM ₃ (O ₂)	6	1.806055000	0.448682000	0.102188000
	6	2.412637000	-0.080904000	1.269001000
	6	3.706203000	-0.608641000	1.245944000
	6	4.429253000	-0.626505000	0.044387000
	6	3.859933000	-0.106188000	-1.126956000
	6	2.568969000	0.426751000	-1.093456000
	1	1.330150000	1.650328000	0.378628000
	1	5.436423000	-1.035899000	0.023116000
	1	4.426467000	-0.110182000	-2.055079000
	1	2.149220000	0.854217000	-2.001896000
	46	-0.376360000	0.254619000	-0.228158000
	8	1.126478000	2.938525000	0.630908000
	6	-0.002203000	3.240530000	0.105311000
	8	-0.793091000	2.385625000	-0.392361000
	6	-0.384483000	4.704941000	0.057651000
	1	-1.453396000	4.820025000	-0.124250000
	1	-0.099800000	5.200215000	0.988404000
	1	0.168310000	5.182682000	-0.758133000
	1	1.872448000	-0.042542000	2.212887000
	1	4.154697000	-0.997376000	2.157091000
	6	-3.259823000	-0.193304000	0.270098000
	8	-2.951586000	-0.501104000	1.436928000
	8	-2.419732000	0.046239000	-0.693430000
	6	-4.722034000	-0.093471000	-0.158162000
	1	-5.383918000	-0.229581000	0.698985000
	1	-4.913910000	0.878353000	-0.622201000
	1	-4.939515000	-0.861049000	-0.908206000
	15	-0.192538000	-2.064557000	-0.075044000
	6	1.273971000	-2.852757000	-0.848842000
	1	2.193096000	-2.497853000	-0.381209000
	1	1.207534000	-3.939394000	-0.731134000
	1	1.303383000	-2.609890000	-1.913911000
	6	-0.207033000	-2.681366000	1.653811000

	1	-0.203171000	-3.776315000	1.659183000
	1	0.670516000	-2.317470000	2.192054000
	1	-1.108772000	-2.310990000	2.146055000
	6	-1.594695000	-2.942872000	-0.871684000
	1	-2.520303000	-2.724467000	-0.338465000
	1	-1.699073000	-2.619347000	-1.909496000
	1	-1.406821000	-4.021234000	-0.843595000
INT-2-PMe₃(O1)	6	1.843913000	-0.365176000	-0.257635000
	6	2.453255000	-1.137806000	0.747606000
	6	3.829730000	-1.414355000	0.706612000
	6	4.613457000	-0.934939000	-0.349278000
	6	4.016107000	-0.171447000	-1.360918000
	6	2.643636000	0.114299000	-1.311753000
	1	1.905482000	1.316797000	1.064765000
	1	5.678160000	-1.153695000	-0.384750000
	1	4.616972000	0.204368000	-2.186850000
	1	2.203001000	0.718278000	-2.103576000
	46	-0.181115000	0.015205000	-0.252987000
	8	1.866131000	2.284083000	1.276300000
	6	0.891613000	2.838921000	0.565652000
	8	0.104996000	2.188639000	-0.138753000
	6	0.827483000	4.333489000	0.682753000
	1	1.734437000	4.766168000	0.249842000
	1	-0.049236000	4.713719000	0.160956000
	1	0.796759000	4.620009000	1.737296000
	1	1.857627000	-1.533393000	1.567667000
	1	4.284233000	-2.007344000	1.497917000
	6	-0.802938000	-2.743674000	0.514732000
	8	-1.033402000	-2.290252000	1.652279000
	8	-0.442209000	-2.045970000	-0.520738000
	6	-0.907655000	-4.242794000	0.241052000
	1	-1.606037000	-4.709044000	0.939444000
	1	-1.214793000	-4.441757000	-0.788252000
	1	0.078900000	-4.696076000	0.389857000
	15	-2.624828000	0.432507000	-0.240800000
	6	-3.720200000	-0.957378000	-0.752748000
	1	-3.573317000	-1.804795000	-0.078569000
	1	-4.773229000	-0.657662000	-0.728493000
	1	-3.460870000	-1.274459000	-1.766461000
	6	-3.299759000	0.917395000	1.405846000
	1	-4.374851000	1.119765000	1.352817000
	1	-3.118890000	0.110922000	2.121242000
	1	-2.785534000	1.815254000	1.760558000
	6	-3.166008000	1.816085000	-1.335403000

	1	-4.241262000	2.002822000	-1.243712000
	1	-2.619361000	2.724499000	-1.068089000
	1	-2.934392000	1.570857000	-2.376022000
INT-2-PMe₃(O₂)	6	1.570128000	-0.576912000	-0.035380000
	6	2.122627000	-0.828893000	1.235753000
	6	3.466866000	-1.216370000	1.378728000
	6	4.278708000	-1.367095000	0.250338000
	6	3.740460000	-1.125215000	-1.021496000
	6	2.401679000	-0.736831000	-1.162000000
	1	2.225937000	1.444150000	0.774115000
	1	5.317613000	-1.669347000	0.357651000
	1	4.364189000	-1.238436000	-1.905983000
	1	2.007982000	-0.555268000	-2.160114000
	46	-0.306747000	0.187680000	-0.254115000
	8	2.375876000	2.418022000	0.722816000
	6	1.398537000	2.973495000	0.000917000
	8	0.446918000	2.337045000	-0.456390000
	6	1.578752000	4.451023000	-0.204063000
	1	0.706777000	4.866474000	-0.706910000
	1	1.732351000	4.944110000	0.759418000
	1	2.473493000	4.624101000	-0.809888000
	1	1.511329000	-0.720085000	2.129926000
	1	3.871450000	-1.398146000	2.372217000
	6	-3.149992000	1.093969000	0.351063000
	8	-3.088800000	0.463079000	1.430356000
	8	-2.242105000	1.100040000	-0.569018000
	6	-4.387833000	1.929992000	0.021196000
	1	-5.075011000	1.964468000	0.869083000
	1	-4.095372000	2.947426000	-0.256308000
	1	-4.905021000	1.495687000	-0.841395000
	15	-1.083446000	-1.982573000	-0.106079000
	6	-2.753780000	-2.181981000	-0.844135000
	1	-3.067086000	-3.228862000	-0.772696000
	1	-3.462978000	-1.551064000	-0.306974000
	1	-2.733261000	-1.881853000	-1.894500000
	6	-1.284501000	-2.564503000	1.623559000
	1	-1.725726000	-3.566789000	1.638132000
	1	-0.312929000	-2.596122000	2.122545000
	1	-1.937643000	-1.863959000	2.148483000
	6	-0.105823000	-3.306878000	-0.924089000
	1	0.887881000	-3.372235000	-0.477171000
	1	-0.617426000	-4.269100000	-0.816331000
	1	0.005436000	-3.078137000	-1.987289000
TS-2-SMe₂(O₁)	6	-1.593298000	0.979611000	0.029194000

	6	-2.336768000	0.686196000	-1.137951000
	6	-3.726284000	0.539711000	-1.094147000
	6	-4.402577000	0.677467000	0.126261000
	6	-3.689766000	0.971034000	1.297765000
	6	-2.300767000	1.116073000	1.246763000
	1	-0.732434000	2.032226000	-0.170695000
	1	-5.483438000	0.562142000	0.163427000
	1	-4.217882000	1.087112000	2.241434000
	1	-1.758863000	1.354663000	2.160084000
	46	0.336795000	-0.035297000	0.185844000
	8	-0.076874000	3.087727000	-0.363218000
	6	1.169247000	2.795970000	-0.325965000
	8	1.611904000	1.625382000	-0.114237000
	6	2.156681000	3.912589000	-0.569787000
	1	3.164418000	3.607147000	-0.288588000
	1	2.140966000	4.164586000	-1.635011000
	1	1.857028000	4.802942000	-0.012871000
	1	-1.822320000	0.586360000	-2.091577000
	1	-4.281792000	0.320056000	-2.003022000
	6	3.511451000	-0.465622000	1.426236000
	1	3.140774000	-0.501513000	2.452311000
	1	4.499049000	-0.931052000	1.380197000
	1	3.554149000	0.568019000	1.080078000
	6	3.142817000	-1.260087000	-1.237389000
	1	4.123980000	-1.740257000	-1.211935000
	1	2.493206000	-1.771608000	-1.948254000
	1	3.238903000	-0.205704000	-1.502627000
	6	-0.752116000	-2.677634000	-0.336639000
	8	-0.098353000	-2.637698000	-1.394178000
	8	-0.794588000	-1.732752000	0.561058000
	6	-1.617045000	-3.883773000	0.015808000
	1	-1.484874000	-4.163630000	1.064263000
	1	-2.671333000	-3.623131000	-0.125438000
	1	-1.371664000	-4.728428000	-0.630539000
	16	2.350837000	-1.430423000	0.398352000
TS-2-SMe ₂ (O ₂)	6	1.831070000	0.497281000	0.104305000
	6	2.382976000	0.096924000	1.346026000
	6	3.662046000	-0.459161000	1.426403000
	6	4.418427000	-0.635574000	0.258444000
	6	3.901721000	-0.240349000	-0.983807000
	6	2.623777000	0.320562000	-1.055988000
	1	1.303251000	1.728303000	0.188688000
	1	5.412283000	-1.073147000	0.317429000
	1	4.496206000	-0.366745000	-1.885559000

	1	2.236911000	0.639100000	-2.022194000
	46	-0.297212000	0.067721000	-0.184962000
	8	0.974382000	2.975446000	0.263102000
	6	-0.249237000	3.073451000	-0.102893000
	8	-0.981643000	2.080369000	-0.391198000
	6	-0.843564000	4.462353000	-0.181750000
	1	-1.843646000	4.432979000	-0.613635000
	1	-0.894091000	4.881319000	0.827903000
	1	-0.192122000	5.107978000	-0.776066000
	1	1.805055000	0.238499000	2.257436000
	1	4.071381000	-0.754396000	2.389619000
	6	-0.482879000	-2.935013000	-1.595907000
	1	0.078863000	-2.583779000	-2.463018000
	1	-0.433145000	-4.025214000	-1.543953000
	1	-1.515459000	-2.587400000	-1.647411000
	6	-0.710260000	-2.981399000	1.196011000
	1	-0.586618000	-4.066560000	1.164829000
	1	-0.350534000	-2.596552000	2.151056000
	1	-1.753868000	-2.704462000	1.051510000
	6	-3.149973000	-0.328702000	0.388213000
	8	-2.874975000	0.011761000	1.551791000
	8	-2.282336000	-0.518660000	-0.567750000
	6	-4.597545000	-0.548455000	-0.042913000
	1	-5.230028000	-0.733120000	0.827810000
	1	-4.956091000	0.355626000	-0.547521000
	1	-4.680122000	-1.377028000	-0.750735000
	16	0.331295000	-2.247088000	-0.112647000
INT-2-SMe ₂ (O1)	6	1.720119000	-0.268800000	-0.252282000
	6	2.337278000	-1.013632000	0.766182000
	6	3.735858000	-1.135717000	0.805121000
	6	4.524636000	-0.531016000	-0.180169000
	6	3.911598000	0.204031000	-1.203180000
	6	2.515850000	0.339358000	-1.237632000
	1	1.506736000	1.392673000	1.224953000
	1	5.606960000	-0.631726000	-0.152791000
	1	4.517033000	0.675576000	-1.974557000
	1	2.058273000	0.922254000	-2.034556000
	46	-0.294304000	-0.080401000	-0.337493000
	8	1.365062000	2.352356000	1.410779000
	6	0.426230000	2.820993000	0.595063000
	8	-0.218244000	2.106732000	-0.186625000
	6	0.216853000	4.302709000	0.700555000
	1	1.119554000	4.816933000	0.357115000
	1	-0.634355000	4.605164000	0.092779000

	1	0.057047000	4.580003000	1.745749000
	1	1.736197000	-1.504962000	1.527567000
	1	4.203105000	-1.708952000	1.603167000
	6	-3.307918000	1.528096000	-1.360330000
	1	-3.077859000	1.333658000	-2.409869000
	1	-4.378071000	1.722609000	-1.256303000
	1	-2.727414000	2.384276000	-1.012110000
	6	-3.324579000	0.533997000	1.267604000
	1	-4.404051000	0.694098000	1.323591000
	1	-3.034988000	-0.286826000	1.925228000
	1	-2.792801000	1.443461000	1.556400000
	6	-0.851911000	-2.842971000	0.402071000
	8	-1.206716000	-2.369472000	1.498826000
	8	-0.386383000	-2.157955000	-0.601093000
	6	-0.920529000	-4.344708000	0.135132000
	1	-1.487330000	-4.849156000	0.919842000
	1	-1.376185000	-4.542741000	-0.839000000
	1	0.095209000	-4.753767000	0.110555000
	16	-2.861232000	0.024909000	-0.424186000
INT-2-SMe ₂ (O ₂)	6	1.628477000	-0.477663000	0.046720000
	6	2.168826000	-0.764785000	1.312743000
	6	3.549680000	-0.976797000	1.468884000
	6	4.400308000	-0.919417000	0.360379000
	6	3.867473000	-0.645222000	-0.906877000
	6	2.492369000	-0.423884000	-1.062683000
	1	1.736096000	1.612904000	0.937021000
	1	5.467876000	-1.087041000	0.480121000
	1	4.521996000	-0.598744000	-1.774799000
	1	2.099519000	-0.201778000	-2.053119000
	46	-0.337215000	-0.039640000	-0.209971000
	8	1.737871000	2.591850000	0.819447000
	6	0.868041000	2.916576000	-0.137425000
	8	0.133027000	2.095592000	-0.696049000
	6	0.869779000	4.378796000	-0.477487000
	1	0.087934000	4.593417000	-1.204181000
	1	0.714742000	4.967813000	0.430483000
	1	1.846426000	4.653535000	-0.886991000
	1	1.521715000	-0.827981000	2.185491000
	1	3.952145000	-1.189786000	2.456877000
	6	-0.198181000	-3.270318000	-1.187635000
	1	0.884128000	-3.161155000	-1.262863000
	1	-0.455300000	-4.323489000	-1.052351000
	1	-0.676303000	-2.872429000	-2.084186000
	6	-2.538717000	-2.607339000	0.194891000

	1	-2.731532000	-3.678706000	0.290669000
	1	-2.985250000	-2.070887000	1.032504000
	1	-2.933525000	-2.220648000	-0.744747000
	6	-3.174200000	0.759488000	0.379577000
	8	-2.860806000	0.670686000	1.587499000
	8	-2.399364000	0.475139000	-0.616447000
	6	-4.579219000	1.211852000	-0.018875000
	1	-5.139349000	1.560926000	0.851029000
	1	-4.525747000	2.008144000	-0.767462000
	1	-5.116881000	0.373402000	-0.475465000
	16	-0.735652000	-2.341745000	0.294485000
TS-2-C ₂ H ₄ (O1)	6	-0.330161000	1.397132000	-0.051403000
	6	-1.314251000	1.591148000	-1.049365000
	6	-2.377171000	2.475042000	-0.849065000
	6	-2.493425000	3.164200000	0.367184000
	6	-1.536883000	2.982500000	1.375609000
	6	-0.466552000	2.108561000	1.164834000
	1	0.936228000	1.512557000	-0.566551000
	1	-3.326143000	3.845364000	0.526475000
	1	-1.624185000	3.524077000	2.314526000
	1	0.284299000	1.992487000	1.944341000
	46	0.433640000	-0.633671000	0.256701000
	8	2.107762000	1.784277000	-0.951089000
	6	2.887766000	0.890996000	-0.470827000
	8	2.480312000	-0.147772000	0.137807000
	6	4.375147000	1.100957000	-0.625860000
	1	4.928534000	0.222427000	-0.295521000
	1	4.605303000	1.323446000	-1.670649000
	1	4.672171000	1.968676000	-0.029113000
	1	-1.236520000	1.053513000	-1.990819000
	1	-3.116396000	2.625683000	-1.632376000
	6	-2.180307000	-1.664116000	-0.516871000
	8	-1.709073000	-1.809138000	-1.655620000
	8	-1.529502000	-1.201493000	0.518840000
	6	-3.634150000	-2.004371000	-0.207505000
	1	-3.735271000	-2.446094000	0.786676000
	1	-4.223094000	-1.080918000	-0.223401000
	1	-4.030210000	-2.684047000	-0.964398000
	6	1.078635000	-2.598811000	1.340593000
	6	1.102806000	-2.864334000	-0.000087000
	1	0.203792000	-2.827570000	1.942493000
	1	1.978077000	-2.290836000	1.867529000
	1	2.021452000	-2.766389000	-0.572584000
	1	0.249821000	-3.303950000	-0.507804000

TS-2-C₂H₄(O2)	6	1.773825000	0.190175000	0.133788000
	6	2.452428000	-0.317359000	1.269503000
	6	3.780492000	-0.740501000	1.189548000
	6	4.458426000	-0.678471000	-0.036952000
	6	3.814433000	-0.175306000	-1.176647000
	6	2.489219000	0.256036000	-1.088654000
	1	1.172165000	1.324686000	0.436628000
	1	5.490608000	-1.014119000	-0.101988000
	1	4.347277000	-0.116994000	-2.122438000
	1	2.002291000	0.663216000	-1.972560000
	46	-0.341816000	-0.314344000	-0.180097000
	8	0.748231000	2.557447000	0.672646000
	6	-0.373494000	2.678066000	0.072903000
	8	-0.998461000	1.707524000	-0.458665000
	6	-0.973837000	4.063252000	-0.030377000
	1	-2.024728000	4.010068000	-0.314493000
	1	-0.860207000	4.589860000	0.919560000
	1	-0.423193000	4.624382000	-0.792346000
	1	1.940429000	-0.348531000	2.229068000
	1	4.289319000	-1.113406000	2.074990000
	6	-3.205641000	-0.773701000	0.224376000
	8	-2.995753000	-0.486868000	1.414359000
	8	-2.287223000	-0.880404000	-0.698635000
	6	-4.619042000	-1.019777000	-0.294422000
	1	-5.288677000	-1.262398000	0.533010000
	1	-4.980140000	-0.106534000	-0.779948000
	1	-4.633928000	-1.819471000	-1.038863000
	6	-0.104732000	-2.393720000	0.672873000
	6	0.270165000	-2.435925000	-0.652122000
	1	-1.122733000	-2.618049000	0.974820000
	1	0.638456000	-2.340320000	1.461879000
	1	1.317290000	-2.417284000	-0.938088000
	1	-0.448471000	-2.693470000	-1.425310000
INT-2-C₂H₄(O1)	6	-0.412206000	1.211876000	-0.250559000
	6	-0.162185000	2.062182000	0.837368000
	6	-0.690307000	3.364367000	0.844070000
	6	-1.449380000	3.824771000	-0.237203000
	6	-1.687830000	2.978517000	-1.328121000
	6	-1.175067000	1.673262000	-1.335498000
	1	-1.990812000	0.397022000	1.045228000
	1	-1.851213000	4.835023000	-0.232261000
	1	-2.275342000	3.329780000	-2.173691000
	1	-1.377820000	1.026271000	-2.186478000
	46	0.310788000	-0.680595000	-0.305914000

	8	-2.784507000	-0.166327000	1.214666000
	6	-2.681325000	-1.289472000	0.512529000
	8	-1.686066000	-1.583009000	-0.164772000
	6	-3.888437000	-2.175691000	0.603114000
	1	-4.732204000	-1.680362000	0.112870000
	1	-3.689207000	-3.129943000	0.118135000
	1	-4.158529000	-2.328370000	1.651079000
	1	0.446371000	1.720890000	1.670379000
	1	-0.498923000	4.015573000	1.694263000
	6	2.927983000	0.361122000	0.491829000
	8	2.575587000	0.120724000	1.660576000
	8	2.211539000	0.145483000	-0.575145000
	6	4.289653000	0.984552000	0.196825000
	1	4.970855000	0.824168000	1.034883000
	1	4.720871000	0.578945000	-0.721658000
	1	4.160347000	2.063329000	0.055025000
	6	1.229544000	-2.922716000	0.232771000
	6	1.140082000	-2.862652000	-1.117229000
	1	2.136225000	-2.634157000	0.756911000
	1	0.426331000	-3.343439000	0.832863000
	1	0.264824000	-3.236357000	-1.643143000
	1	1.976409000	-2.526663000	-1.724355000
INT-2-C ₂ H ₄ (O ₂)	6	1.608125000	-0.535671000	0.001804000
	6	2.164756000	-0.575108000	1.291057000
	6	3.555147000	-0.459570000	1.466255000
	6	4.394573000	-0.317778000	0.356921000
	6	3.841964000	-0.288333000	-0.930663000
	6	2.456034000	-0.397917000	-1.109431000
	1	1.374408000	1.630416000	0.824991000
	1	5.469857000	-0.232495000	0.492086000
	1	4.488391000	-0.178131000	-1.798652000
	1	2.045076000	-0.367081000	-2.116331000
	46	-0.402583000	-0.548640000	-0.239051000
	8	1.135429000	2.577079000	0.696131000
	6	0.126210000	2.664654000	-0.172662000
	8	-0.438031000	1.681938000	-0.662035000
	6	-0.256947000	4.079303000	-0.498208000
	1	-1.092069000	4.087833000	-1.196621000
	1	-0.531477000	4.602828000	0.421987000
	1	0.601944000	4.600241000	-0.930757000
	1	1.529508000	-0.692782000	2.167105000
	1	3.972736000	-0.484126000	2.470254000
	6	-3.239800000	-0.122827000	0.442711000
	8	-2.759427000	0.235245000	1.540934000

	8	-2.546830000	-0.567388000	-0.557534000
	6	-4.743951000	-0.039450000	0.193230000
	1	-5.282226000	0.162550000	1.121480000
	1	-4.948609000	0.768648000	-0.517765000
	1	-5.111482000	-0.967316000	-0.254833000
	6	-0.301288000	-2.666959000	-0.937126000
	6	-0.514772000	-2.668754000	0.429219000
	1	-1.137880000	-2.711516000	-1.629634000
	1	0.687943000	-2.846517000	-1.347783000
	1	0.304351000	-2.851695000	1.118677000
	1	-1.521093000	-2.727954000	0.833555000
TS-2-C ₂ H ₂ (O1)	6	-0.165179000	1.426308000	0.029933000
	6	-0.857596000	1.760958000	-1.159148000
	6	-1.929589000	2.656285000	-1.139939000
	6	-2.338009000	3.227029000	0.074024000
	6	-1.668889000	2.911519000	1.266143000
	6	-0.599716000	2.014472000	1.243153000
	1	1.165564000	1.553055000	-0.123205000
	1	-3.174583000	3.921687000	0.090933000
	1	-1.982611000	3.365196000	2.203207000
	1	-0.079241000	1.782643000	2.170134000
	46	0.398801000	-0.671009000	0.200465000
	8	2.416482000	1.797056000	-0.282509000
	6	3.037069000	0.680255000	-0.260000000
	8	2.470236000	-0.444361000	-0.088217000
	6	4.536409000	0.707349000	-0.450601000
	1	4.951500000	-0.299482000	-0.417976000
	1	4.767410000	1.176189000	-1.411083000
	1	4.986010000	1.322382000	0.333938000
	1	-0.538942000	1.331539000	-2.106216000
	1	-2.445965000	2.910360000	-2.062461000
	6	-2.304114000	-1.540784000	-0.368209000
	8	-1.872556000	-1.863845000	-1.487369000
	8	-1.600371000	-0.983817000	0.581515000
	6	-3.753621000	-1.791044000	0.033491000
	1	-3.788635000	-2.565928000	0.806235000
	1	-4.195535000	-0.884800000	0.456197000
	1	-4.333732000	-2.119900000	-0.830319000
	6	0.966760000	-2.821741000	1.028238000
	6	0.641831000	-3.000102000	-0.136724000
	1	1.289527000	-2.792925000	2.053155000
	1	0.331923000	-3.256884000	-1.133462000
TS-2-C ₂ H ₂ (O2)	6	1.751816000	0.117244000	0.078009000
	6	2.236721000	-0.385863000	1.310456000

	6	3.470455000	-1.034675000	1.389921000
	6	4.241952000	-1.205306000	0.230803000
	6	3.787349000	-0.715277000	-1.002398000
	6	2.554666000	-0.063168000	-1.075387000
	1	1.348024000	1.369751000	0.200307000
	1	5.200543000	-1.715236000	0.289718000
	1	4.395040000	-0.839768000	-1.895239000
	1	2.214235000	0.329439000	-2.031563000
	46	-0.388688000	-0.160027000	-0.247365000
	8	1.100254000	2.652662000	0.330291000
	6	-0.138525000	2.830897000	0.077255000
	8	-0.950322000	1.893586000	-0.201679000
	6	-0.667076000	4.248363000	0.116450000
	1	-1.716587000	4.280259000	-0.174513000
	1	-0.552289000	4.642152000	1.130462000
	1	-0.071331000	4.875596000	-0.551928000
	1	1.646433000	-0.247288000	2.214038000
	1	3.833394000	-1.405839000	2.345161000
	6	-3.145420000	-0.953453000	0.320837000
	8	-2.735187000	-1.180467000	1.473827000
	8	-2.413459000	-0.516061000	-0.664217000
	6	-4.600557000	-1.202047000	-0.064930000
	1	-4.657502000	-2.091710000	-0.701245000
	1	-5.208016000	-1.364438000	0.827227000
	1	-4.997720000	-0.360883000	-0.639226000
	6	-0.173290000	-2.369725000	0.210656000
	6	0.098002000	-2.255803000	-0.982187000
	1	-0.427000000	-2.629754000	1.222820000
	1	0.365565000	-2.345907000	-2.019895000
INT-2-C ₂ H ₂ (O1)	6	-0.498448000	1.186252000	-0.253612000
	6	-0.186883000	2.060222000	0.797970000
	6	-0.800634000	3.322151000	0.860650000
	6	-1.705972000	3.717505000	-0.130288000
	6	-2.005216000	2.845824000	-1.185265000
	6	-1.407029000	1.578780000	-1.247848000
	1	-1.835274000	0.120927000	1.278957000
	1	-2.174304000	4.697527000	-0.082829000
	1	-2.706359000	3.146920000	-1.960640000
	1	-1.657278000	0.908861000	-2.067401000
	46	0.338307000	-0.639441000	-0.367509000
	8	-2.599167000	-0.484627000	1.426024000
	6	-2.551068000	-1.474776000	0.539212000
	8	-1.619152000	-1.629114000	-0.261929000
	6	-3.738816000	-2.389509000	0.587890000

	1	-4.626682000	-1.839069000	0.261790000
	1	-3.576730000	-3.246944000	-0.063203000
	1	-3.912362000	-2.717423000	1.615873000
	1	0.530384000	1.770621000	1.561570000
	1	-0.561971000	3.993528000	1.682629000
	6	2.974160000	0.367846000	0.422422000
	8	2.734821000	-0.133441000	1.538798000
	8	2.176109000	0.336514000	-0.604514000
	6	4.280859000	1.110512000	0.159944000
	1	5.003023000	0.907372000	0.952857000
	1	4.699763000	0.828530000	-0.809578000
	1	4.080302000	2.187004000	0.130899000
	6	1.675982000	-2.698808000	0.106928000
	6	1.096391000	-3.006024000	-0.918531000
	1	2.226964000	-2.420083000	0.988304000
	1	0.607575000	-3.357998000	-1.807677000
INT-2-C ₂ H ₂ (O ₂)	6	1.589217000	-0.597756000	-0.084209000
	6	2.139770000	-1.023490000	1.134105000
	6	3.534474000	-1.058992000	1.302109000
	6	4.380082000	-0.692111000	0.250166000
	6	3.830177000	-0.281905000	-0.971776000
	6	2.439379000	-0.232431000	-1.140273000
	1	1.343215000	1.358643000	1.122375000
	1	5.458986000	-0.727357000	0.378760000
	1	4.481466000	0.002532000	-1.795321000
	1	2.028252000	0.096361000	-2.092524000
	46	-0.411872000	-0.417119000	-0.328374000
	8	1.208036000	2.334177000	1.105657000
	6	0.351573000	2.644999000	0.133216000
	8	-0.237564000	1.802081000	-0.553516000
	6	0.177007000	4.122573000	-0.062374000
	1	-0.658326000	4.313825000	-0.734041000
	1	0.014862000	4.610993000	0.901415000
	1	1.096223000	4.533134000	-0.492191000
	1	1.496120000	-1.331604000	1.955048000
	1	3.951837000	-1.381231000	2.253430000
	6	-3.384369000	-0.255745000	0.317890000
	8	-3.103909000	-0.632067000	1.479837000
	8	-2.538685000	-0.120228000	-0.651317000
	6	-4.826513000	0.094766000	-0.047303000
	1	-5.505714000	-0.136848000	0.775542000
	1	-4.895306000	1.163094000	-0.279056000
	1	-5.134014000	-0.451434000	-0.944271000
	6	-0.261163000	-2.657469000	-0.636629000

	6	-0.975444000	-2.475045000	0.349722000
	1	0.353269000	-3.049991000	-1.426960000
	1	-1.672901000	-2.408721000	1.169848000
TS-2-NHC(O1)	6	-2.173592000	0.369235000	0.103166000
	6	-2.803694000	0.097226000	-1.132042000
	6	-4.036338000	-0.564036000	-1.199570000
	6	-4.678087000	-0.964430000	-0.019899000
	6	-4.085132000	-0.695286000	1.221862000
	6	-2.850825000	-0.038270000	1.274651000
	1	-1.751020000	1.737668000	0.207452000
	1	-5.636235000	-1.477497000	-0.067389000
	1	-4.585359000	-0.996099000	2.140228000
	1	-2.408104000	0.166727000	2.248747000
	46	0.051315000	0.222749000	0.116718000
	8	-1.601127000	2.930514000	0.262440000
	6	-0.353627000	3.189170000	0.082372000
	8	0.531913000	2.296491000	-0.049827000
	6	0.044605000	4.643602000	0.027936000
	1	-0.484985000	5.132157000	-0.794871000
	1	-0.261347000	5.136941000	0.954772000
	1	1.120685000	4.745534000	-0.110039000
	1	-2.326521000	0.411673000	-2.059191000
	1	-4.496865000	-0.765236000	-2.164693000
	6	-0.121048000	-2.622950000	-0.595321000
	8	0.187471000	-2.297407000	-1.754567000
	8	-0.252709000	-1.813926000	0.417518000
	6	-0.411315000	-4.080331000	-0.238865000
	1	-0.094405000	-4.741506000	-1.047628000
	1	0.091826000	-4.361083000	0.690488000
	1	-1.487811000	-4.204547000	-0.080436000
	6	2.094789000	-0.138785000	0.121700000
	6	4.167272000	-0.771820000	0.761539000
	6	4.265214000	-0.255601000	-0.494251000
	1	4.921311000	-1.178093000	1.419849000
	1	5.119030000	-0.135953000	-1.145106000
	7	2.984228000	0.131034000	-0.867289000
	7	2.827111000	-0.696444000	1.119770000
	6	2.305219000	-1.098552000	2.427838000
	1	2.829494000	-1.996195000	2.761258000
	1	2.456051000	-0.299362000	3.158590000
	1	1.243750000	-1.318974000	2.330530000
	6	2.650915000	0.677410000	-2.183696000
	1	2.667921000	-0.115747000	-2.935226000
	1	1.656483000	1.116807000	-2.142293000

	1	3.375698000	1.449352000	-2.450489000
TS-2-NHC(O2)	6	-1.637032000	0.910112000	-0.036175000
	6	-2.043459000	1.126995000	-1.376522000
	6	-3.334441000	0.812652000	-1.811170000
	6	-4.262598000	0.276751000	-0.907602000
	6	-3.896224000	0.063266000	0.428979000
	6	-2.600866000	0.372769000	0.852200000
	1	-1.027144000	2.000500000	0.495418000
	1	-5.269254000	0.035312000	-1.241060000
	1	-4.619879000	-0.339596000	1.133923000
	1	-2.337210000	0.217407000	1.896265000
	46	0.486753000	0.352939000	0.125142000
	8	-0.641410000	3.185602000	0.850572000
	6	0.562334000	3.325736000	0.422581000
	8	1.249411000	2.372827000	-0.047178000
	6	1.163445000	4.712093000	0.485702000
	1	2.205205000	4.697802000	0.165026000
	1	0.588147000	5.383971000	-0.158228000
	1	1.092808000	5.095032000	1.507538000
	1	-1.340662000	1.563981000	-2.083454000
	1	-3.620940000	0.989240000	-2.845411000
	6	3.126524000	-0.653932000	-0.761350000
	8	2.636532000	-0.716438000	-1.906211000
	8	2.493535000	-0.301171000	0.316265000
	6	4.601339000	-0.980105000	-0.529406000
	1	5.012970000	-1.525322000	-1.381044000
	1	5.158282000	-0.044145000	-0.410358000
	1	4.734682000	-1.560238000	0.387541000
	6	-0.116703000	-1.565543000	0.331227000
	6	-0.737748000	-3.684790000	-0.117980000
	6	-0.633074000	-3.567789000	1.233939000
	1	-1.004105000	-4.530877000	-0.734244000
	1	-0.787976000	-4.290538000	2.021582000
	7	-0.249573000	-2.257359000	1.491576000
	7	-0.412371000	-2.446145000	-0.656352000
	6	-0.415833000	-2.137669000	-2.090642000
	1	-0.337922000	-3.072813000	-2.647309000
	1	-1.343539000	-1.629513000	-2.363087000
	1	0.444007000	-1.506462000	-2.318573000
	6	-0.005807000	-1.731740000	2.835468000
	1	-0.918900000	-1.796988000	3.432077000
	1	0.787075000	-2.306259000	3.319875000
	1	0.303664000	-0.690557000	2.757330000
INT-2-NHC(O1)	6	-2.048556000	-0.190972000	0.292086000

	6	-2.766537000	-1.058213000	-0.554124000
	6	-4.158193000	-1.201629000	-0.434913000
	6	-4.859758000	-0.489112000	0.545087000
	6	-4.161470000	0.374549000	1.398988000
	6	-2.773043000	0.524306000	1.266736000
	1	-1.819445000	1.319347000	-1.248130000
	1	-5.936943000	-0.604517000	0.642657000
	1	-4.696070000	0.933438000	2.165038000
	1	-2.255816000	1.211976000	1.935102000
	46	0.010724000	-0.006647000	0.231184000
	8	-1.710468000	2.267222000	-1.517816000
	6	-0.791295000	2.823910000	-0.735780000
	8	-0.109677000	2.181429000	0.075692000
	6	-0.654976000	4.307401000	-0.915315000
	1	-1.566926000	4.795340000	-0.557687000
	1	0.203287000	4.675409000	-0.355227000
	1	-0.548477000	4.544913000	-1.976843000
	1	-2.238145000	-1.632528000	-1.311907000
	1	-4.691121000	-1.873638000	-1.105286000
	6	0.270148000	-2.822151000	-0.561969000
	8	0.313867000	-2.408668000	-1.738216000
	8	0.134912000	-2.086281000	0.497679000
	6	0.341605000	-4.320012000	-0.267966000
	1	0.850117000	-4.844241000	-1.080046000
	1	0.846696000	-4.516817000	0.680711000
	1	-0.678596000	-4.712867000	-0.191089000
	6	2.168211000	0.164671000	0.241232000
	6	4.334970000	0.330828000	-0.416951000
	6	4.314042000	0.424244000	0.941326000
	1	5.160920000	0.357998000	-1.113123000
	1	5.116910000	0.545489000	1.654198000
	7	2.981796000	0.320143000	1.322092000
	7	3.016573000	0.167828000	-0.823329000
	6	2.594076000	0.063304000	-2.221803000
	1	2.432057000	1.058362000	-2.646722000
	1	3.372410000	-0.446242000	-2.793672000
	1	1.675503000	-0.522296000	-2.267683000
	6	2.529220000	0.372324000	2.711364000
	1	3.029980000	-0.401799000	3.298132000
	1	2.748144000	1.352418000	3.143511000
	1	1.453891000	0.199931000	2.735582000
INT-2-NHC(O2)	6	1.473613000	-0.834551000	0.025406000
	6	1.856842000	-1.266001000	1.311454000
	6	3.039055000	-1.998707000	1.514357000

	6	3.857727000	-2.329064000	0.429801000
	6	3.488067000	-1.916675000	-0.857801000
	6	2.312175000	-1.180431000	-1.055142000
	1	2.435220000	1.005598000	0.864277000
	1	4.770815000	-2.899323000	0.583264000
	1	4.117349000	-2.165567000	-1.710198000
	1	2.056899000	-0.866220000	-2.065317000
	46	-0.156112000	0.356232000	-0.297056000
	8	2.817256000	1.914459000	0.807777000
	6	2.091460000	2.638764000	-0.046402000
	8	1.068364000	2.218356000	-0.593447000
	6	2.644554000	4.014885000	-0.282463000
	1	1.967964000	4.584268000	-0.917834000
	1	2.785624000	4.525650000	0.673816000
	1	3.625130000	3.933521000	-0.761072000
	1	1.238388000	-1.029658000	2.174797000
	1	3.312987000	-2.310130000	2.520414000
	6	-2.472504000	2.248694000	0.179698000
	8	-2.176900000	2.196361000	1.396186000
	8	-1.883025000	1.599816000	-0.768137000
	6	-3.629214000	3.136237000	-0.286632000
	1	-4.056381000	3.696785000	0.547503000
	1	-3.281500000	3.833822000	-1.055359000
	1	-4.409932000	2.517360000	-0.741805000
	6	-1.264498000	-1.327138000	-0.077032000
	6	-2.366337000	-3.254810000	-0.500687000
	6	-2.593829000	-2.929175000	0.800555000
	1	-2.718344000	-4.086031000	-1.093962000
	1	-3.180493000	-3.424645000	1.560286000
	7	-1.914726000	-1.741345000	1.041817000
	7	-1.549884000	-2.259605000	-1.023573000
	6	-1.080488000	-2.239942000	-2.408689000
	1	-0.370615000	-3.053396000	-2.578323000
	1	-1.930469000	-2.349857000	-3.085990000
	1	-0.591669000	-1.285833000	-2.598373000
	6	-1.896145000	-1.057693000	2.337905000
	1	-2.868318000	-1.185372000	2.818343000
	1	-1.121362000	-1.485274000	2.980240000
	1	-1.716285000	0.005962000	2.177164000

Table S4. Cartesian coordinates of the optimized stationary points involved in the Heck coupling reaction designed, calculated at the B3LYP/DGDZVP level of theory in CH₂Cl₂ solvent.

Names	Cartesian Coordinates			
pre-COM	6	1.668301000	-0.167886000	0.166592000
	6	2.515959000	-0.134494000	-0.945520000
	6	3.865730000	-0.488875000	-0.800878000
	6	4.365860000	-0.869617000	0.450609000
	6	3.513574000	-0.895177000	1.560277000
	6	2.161702000	-0.540962000	1.422109000
	1	4.521904000	-0.465842000	-1.668185000
	1	5.412759000	-1.141821000	0.559978000
	1	3.893859000	-1.186722000	2.536860000
	1	1.512665000	-0.566420000	2.295212000
	46	-0.310254000	0.146267000	-0.092772000
	6	-0.188502000	2.390439000	-0.068023000
	6	-0.239180000	1.927756000	1.240209000
	1	0.653513000	1.905651000	1.856459000
	1	-4.904111000	1.347716000	-0.358808000
	6	-4.735878000	0.368280000	0.099432000
	6	-3.265677000	0.208971000	0.479908000
	1	-5.380597000	0.256009000	0.973271000
	1	-5.005878000	-0.387763000	-0.645614000
	8	-2.431241000	0.434196000	-0.487065000
	8	-2.942260000	-0.118317000	1.642614000
	1	-1.198666000	1.805801000	1.733076000
	1	2.143700000	0.160611000	-1.924504000
	6	1.004646000	2.933496000	-0.664115000
	7	1.930133000	3.424595000	-1.175021000
	1	-1.108626000	2.621941000	-0.600125000
	8	-0.443253000	-2.052769000	-0.741742000
	6	-1.422099000	-2.343218000	-1.759298000
	1	-2.432031000	-2.346202000	-1.337193000
	1	-1.343424000	-1.562790000	-2.515812000
	1	-1.197062000	-3.318687000	-2.204796000
	6	-0.421111000	-3.057390000	0.291523000
	1	-0.230374000	-4.037941000	-0.158561000
	1	0.391265000	-2.802248000	0.971480000
	1	-1.374058000	-3.074547000	0.832495000
TS-3	6	1.635381000	-0.265304000	0.185850000
	6	2.444820000	-0.462228000	-0.940843000
	6	3.836387000	-0.569765000	-0.794462000
	6	4.422884000	-0.483663000	0.474676000

	6	3.612557000	-0.285138000	1.598686000
	6	2.220623000	-0.168490000	1.455500000
	1	4.458892000	-0.719423000	-1.674228000
	1	5.501396000	-0.566652000	0.585562000
	1	4.057968000	-0.215953000	2.588983000
	1	1.607664000	-0.005762000	2.340114000
	46	-0.359149000	-0.259578000	-0.023034000
	6	-0.145518000	2.674612000	-0.692213000
	6	-0.194948000	1.876648000	0.410186000
	1	0.471313000	2.148239000	1.229973000
	1	-5.094587000	-0.572103000	0.100709000
	6	-4.763432000	0.386341000	0.501534000
	6	-3.254167000	0.498817000	0.447884000
	1	-5.201696000	1.197622000	-0.088394000
	1	-5.109912000	0.504949000	1.531351000
	8	-2.585233000	-0.369429000	-0.180479000
	8	-2.728503000	1.509350000	1.049913000
	1	-1.455958000	1.545900000	0.749948000
	1	2.006331000	-0.535663000	-1.933930000
	6	0.732132000	3.805512000	-0.806592000
	7	1.445184000	4.725249000	-0.910613000
	1	-0.796176000	2.509986000	-1.549862000
	8	-0.267202000	-2.467788000	-0.585192000
	6	-1.209161000	-2.904992000	-1.582699000
	1	-2.217153000	-2.974716000	-1.161149000
	1	-1.196300000	-2.164725000	-2.382978000
	1	-0.895961000	-3.879417000	-1.974577000
	6	-0.137522000	-3.411652000	0.493673000
	1	0.172036000	-4.384703000	0.095153000
	1	0.631026000	-3.026911000	1.164256000
	1	-1.087021000	-3.518072000	1.031885000
INT-3	6	1.870025000	0.009807000	0.058734000
	6	2.592604000	-0.211078000	-1.127361000
	6	3.995009000	-0.169624000	-1.131819000
	6	4.698678000	0.098467000	0.049377000
	6	3.987804000	0.330022000	1.233029000
	6	2.584547000	0.295215000	1.234865000
	1	4.535611000	-0.344865000	-2.060124000
	1	5.785751000	0.131727000	0.045637000
	1	4.522042000	0.543816000	2.156897000
	1	2.055825000	0.492041000	2.165403000
	46	-0.134824000	-0.277094000	0.061286000
	6	-0.459701000	2.662058000	-0.637366000
	6	-0.165534000	1.723275000	0.299420000

	1	0.047678000	2.098635000	1.305176000
	1	-4.759055000	-1.728631000	0.198976000
	6	-4.794825000	-0.640467000	0.179033000
	6	-3.402206000	-0.080530000	0.119720000
	1	-5.363943000	-0.299613000	-0.690620000
	1	-5.302903000	-0.265089000	1.071822000
	8	-2.385942000	-0.778828000	0.090428000
	8	-3.369147000	1.254279000	0.100936000
	1	-2.429831000	1.555508000	0.053089000
	1	2.070273000	-0.421137000	-2.058635000
	6	-0.502087000	4.065891000	-0.329081000
	7	-0.543541000	5.209335000	-0.087634000
	1	-0.655553000	2.413975000	-1.679414000
	8	0.057016000	-2.581043000	-0.154372000
	6	-0.528533000	-3.162250000	-1.329858000
	1	-1.621926000	-3.176680000	-1.253068000
	1	-0.226504000	-2.543943000	-2.176592000
	1	-0.152333000	-4.183064000	-1.467552000
	6	-0.220954000	-3.345694000	1.029648000
	1	0.152074000	-4.369676000	0.908005000
	1	0.303082000	-2.860859000	1.854428000
	1	-1.297976000	-3.366984000	1.234869000
TS-4	6	-1.790868000	0.001577000	-0.065195000
	6	-2.480075000	-0.052780000	1.165409000
	6	-3.842760000	-0.359152000	1.209827000
	6	-4.554440000	-0.599058000	0.024017000
	6	-3.889259000	-0.527037000	-1.204685000
	6	-2.521083000	-0.223479000	-1.249385000
	1	-4.354201000	-0.404184000	2.169125000
	1	-5.616646000	-0.828715000	0.060103000
	1	-4.432630000	-0.703215000	-2.130662000
	1	-2.024223000	-0.158187000	-2.215007000
	46	0.251975000	-0.331746000	-0.072681000
	6	-0.387258000	2.559029000	0.569792000
	6	-0.468302000	1.536985000	-0.340486000
	1	-0.612048000	1.840591000	-1.380562000
	1	5.138713000	-0.551723000	-0.211622000
	6	4.837202000	0.494143000	-0.174975000
	6	3.340563000	0.594561000	-0.087718000
	1	5.295704000	0.991530000	0.683737000
	1	5.181440000	1.009846000	-1.076636000
	8	2.581962000	-0.373827000	-0.164411000
	8	2.904970000	1.848788000	0.075387000
	1	1.918413000	1.847908000	0.112671000

	1	-1.952497000	0.155011000	2.093795000
	6	-0.495862000	3.929195000	0.181092000
	7	-0.570297000	5.056483000	-0.129577000
	1	-0.296866000	2.379539000	1.639311000
	8	0.518040000	-2.693852000	0.219777000
	6	1.301602000	-3.130872000	1.337359000
	1	2.371774000	-2.986828000	1.144821000
	1	0.999881000	-2.528136000	2.195764000
	1	1.104933000	-4.190105000	1.546478000
	6	0.795855000	-3.448216000	-0.966427000
	1	0.588194000	-4.512366000	-0.796368000
	1	0.137197000	-3.068776000	-1.749402000
	1	1.842441000	-3.325491000	-1.272948000
INT-4	6	-2.397401000	-0.353854000	0.195044000
	6	-2.769470000	-0.777514000	-1.099281000
	6	-3.883280000	-0.231824000	-1.739716000
	6	-4.654505000	0.755899000	-1.110052000
	6	-4.297317000	1.188115000	0.172475000
	6	-3.184924000	0.637474000	0.815844000
	1	-4.150850000	-0.575477000	-2.736206000
	1	-5.519802000	1.180226000	-1.612948000
	1	-4.887050000	1.951455000	0.674524000
	1	-2.920501000	0.978123000	1.814968000
	46	0.627516000	-0.396261000	-0.051913000
	6	-0.534598000	-2.089108000	0.570064000
	6	-1.229090000	-0.895688000	0.925574000
	1	-1.179338000	-0.590795000	1.970138000
	1	1.902864000	4.376611000	-0.352908000
	6	1.662812000	4.075990000	0.665884000
	6	1.305333000	2.617432000	0.699078000
	1	2.515125000	4.263630000	1.324733000
	1	0.821259000	4.666287000	1.039980000
	8	1.256938000	1.888692000	-0.291500000
	8	1.033079000	2.163913000	1.932385000
	1	0.800182000	1.206945000	1.844424000
	1	-2.183106000	-1.532690000	-1.615910000
	6	0.174607000	-2.838665000	1.565282000
	7	0.748887000	-3.472033000	2.365747000
	1	-0.846346000	-2.683814000	-0.286532000
	8	2.652801000	-0.859148000	-1.321702000
	6	3.875251000	-0.850975000	-0.576720000
	1	4.174674000	0.174699000	-0.323981000
	1	3.696770000	-1.416097000	0.339715000
	1	4.677434000	-1.330535000	-1.152825000

	6	2.776123000	-0.179080000	-2.576059000
	1	3.557307000	-0.648351000	-3.188271000
	1	1.813834000	-0.265695000	-3.083969000
	1	3.015822000	0.880845000	-2.425133000
TS-3'	6	-1.805547000	0.493122000	-0.257237000
	6	-2.520147000	0.758125000	0.920694000
	6	-3.874412000	0.410405000	1.002416000
	6	-4.520895000	-0.171808000	-0.095680000
	6	-3.810190000	-0.406052000	-1.279511000
	6	-2.454380000	-0.064608000	-1.367674000
	1	-4.423760000	0.603833000	1.920764000
	1	-5.574615000	-0.431255000	-0.032702000
	1	-4.308699000	-0.849690000	-2.138166000
	1	-1.913783000	-0.243112000	-2.294435000
	46	0.236356000	0.090785000	-0.017485000
	6	0.814791000	2.071738000	-0.512443000
	6	-0.552348000	2.151489000	-0.880470000
	1	-1.218376000	2.785492000	-0.309481000
	1	4.917837000	-0.234802000	0.760211000
	6	4.536532000	-0.913035000	-0.010598000
	6	3.169779000	-0.422897000	-0.484267000
	1	5.245910000	-0.945597000	-0.839574000
	1	4.450426000	-1.904683000	0.443074000
	8	2.235860000	-0.519713000	0.413343000
	8	3.023033000	0.032737000	-1.637113000
	1	-0.796742000	2.032461000	-1.929631000
	1	-2.031757000	1.228498000	1.771208000
	6	1.287837000	2.742092000	0.671934000
	7	1.686165000	3.302367000	1.614901000
	1	1.573809000	1.871857000	-1.267469000
	8	-0.372530000	-2.078880000	0.495788000
	6	-0.085364000	-2.452948000	1.856226000
	1	0.996079000	-2.489946000	2.025113000
	1	-0.536700000	-1.695135000	2.498142000
	1	-0.533430000	-3.430348000	2.069517000
	6	0.104932000	-3.057571000	-0.445118000
	1	-0.350590000	-4.030301000	-0.226120000
	1	-0.202150000	-2.723459000	-1.437054000
	1	1.196558000	-3.137947000	-0.399186000
INT-3'	6	-1.814806000	1.277339000	-0.486435000
	6	-2.176848000	0.870103000	0.822015000
	6	-3.113968000	-0.163192000	1.015180000
	6	-3.687818000	-0.798838000	-0.082342000
	6	-3.325395000	-0.414510000	-1.387025000

	6	-2.397788000	0.603080000	-1.587907000
	1	-3.392647000	-0.450317000	2.025304000
	1	-4.419062000	-1.589074000	0.065864000
	1	-3.776363000	-0.909167000	-2.243278000
	1	-2.130899000	0.905578000	-2.597483000
	46	0.136413000	0.053121000	0.138312000
	6	0.523593000	2.020807000	-0.279419000
	6	-0.886457000	2.480443000	-0.687967000
	1	-1.231461000	3.329846000	-0.092029000
	1	4.874132000	0.088699000	0.079745000
	6	4.402754000	-0.740273000	-0.459074000
	6	2.940952000	-0.391487000	-0.732569000
	1	4.939859000	-0.905255000	-1.394886000
	1	4.477440000	-1.627295000	0.175814000
	8	2.190384000	-0.426230000	0.330387000
	8	2.559844000	-0.091349000	-1.879374000
	1	-0.889219000	2.783078000	-1.737208000
	1	-1.813843000	1.426568000	1.683022000
	6	1.082027000	2.634015000	0.899437000
	7	1.521767000	3.137182000	1.859139000
	1	1.249256000	1.978656000	-1.092504000
	8	-0.380425000	-2.159532000	0.559196000
	6	0.164497000	-2.645382000	1.798537000
	1	1.256936000	-2.705335000	1.742861000
	1	-0.126735000	-1.936848000	2.575003000
	1	-0.254891000	-3.632902000	2.023619000
	6	-0.119944000	-3.053362000	-0.536293000
	1	-0.539160000	-4.041991000	-0.315348000
	1	-0.611273000	-2.633421000	-1.414874000
	1	0.957365000	-3.140221000	-0.718457000
TS-4'	6	-2.492715000	-0.128570000	-0.314941000
	6	-2.439365000	-0.382778000	1.070828000
	6	-3.521390000	-0.044904000	1.884025000
	6	-4.665686000	0.551506000	1.334157000
	6	-4.722241000	0.812968000	-0.039191000
	6	-3.640269000	0.477599000	-0.857859000
	1	-3.473627000	-0.243860000	2.951488000
	1	-5.504619000	0.812701000	1.974071000
	1	-5.604572000	1.276565000	-0.472194000
	1	-3.687020000	0.684381000	-1.924738000
	46	0.683897000	0.315161000	-0.560027000
	6	-0.403930000	-1.477621000	-0.941747000
	6	-1.401803000	-0.508835000	-1.241506000
	1	-0.417869000	0.986512000	-1.485275000

	1	3.762184000	-2.474612000	1.745126000
	6	3.146420000	-1.862664000	2.412201000
	6	1.934712000	-1.330343000	1.649549000
	1	2.835208000	-2.462344000	3.269499000
	1	3.769026000	-1.029998000	2.754402000
	8	2.234632000	-0.576620000	0.637693000
	8	0.776870000	-1.630923000	2.012755000
	1	-1.617744000	-0.342832000	-2.293455000
	1	-1.551849000	-0.828039000	1.514252000
	6	0.254355000	-2.176930000	-2.013288000
	7	0.781072000	-2.770955000	-2.868991000
	1	-0.402940000	-1.993359000	0.015786000
	8	1.755289000	2.290413000	-0.316129000
	6	3.060449000	2.308541000	-0.929871000
	1	3.740392000	1.629429000	-0.405207000
	1	2.930835000	1.983408000	-1.962948000
	1	3.456424000	3.329930000	-0.909686000
	6	1.785260000	2.788872000	1.036439000
	1	2.194047000	3.805536000	1.039180000
	1	0.754963000	2.804560000	1.393834000
	1	2.393296000	2.137301000	1.672716000
INT-4'	6	-2.257616000	0.541307000	0.074730000
	6	-2.471165000	-0.718632000	-0.526084000
	6	-3.515159000	-1.532137000	-0.087763000
	6	-4.358940000	-1.110624000	0.950717000
	6	-4.154562000	0.136553000	1.553355000
	6	-3.112234000	0.956298000	1.117812000
	1	-3.675773000	-2.499213000	-0.557135000
	1	-5.171548000	-1.750468000	1.285150000
	1	-4.806421000	0.469442000	2.356522000
	1	-2.955981000	1.925564000	1.585706000
	46	0.855717000	0.622372000	0.266458000
	6	-0.326278000	1.304577000	-1.438689000
	6	-1.207578000	1.471555000	-0.357002000
	1	0.804915000	2.044025000	0.882667000
	1	2.703242000	-3.274700000	-1.632837000
	6	1.618620000	-3.363632000	-1.747060000
	6	0.955907000	-1.998010000	-1.567132000
	1	1.385199000	-3.785950000	-2.726241000
	1	1.264592000	-4.046884000	-0.967580000
	8	1.279195000	-1.388335000	-0.474792000
	8	0.162684000	-1.571571000	-2.438627000
	1	-1.275873000	2.465615000	0.075603000
	1	-1.819085000	-1.061202000	-1.324819000

	6	0.335756000	2.441423000	-2.019501000
	7	0.861284000	3.346366000	-2.536431000
	1	-0.350606000	0.408766000	-2.063273000
	8	2.198384000	0.095550000	2.000507000
	6	3.610540000	0.248583000	1.752280000
	1	3.971343000	-0.534842000	1.076862000
	1	3.751819000	1.229172000	1.297010000
	1	4.152264000	0.199565000	2.703259000
	6	1.895536000	-1.144437000	2.673719000
	1	2.470750000	-1.195587000	3.604687000
	1	0.828719000	-1.132092000	2.899225000
	1	2.131384000	-1.996984000	2.030169000

Table S5. Electronic energies (in a.u.) and Gibbs free energies (in a.u.) calculated at the B3LYP/DGDZVP level of theory in CH₂Cl₂ solvent, and electronic energies (in a.u.) by the B3LYP/Def2TZVPP single point calculations in CH₂Cl₂ solvent.

Names	E^{DZVP}	G^{DZVP}	E^{TZVP}
Benzene	-232.2685255	-232.19404	-232.3466638
CAT	-5551.840448	-5551.704737	-740.2882852
TS-1(O1)	-5784.099064	-5783.873764	-972.6294175
INT-1(O1)	-5784.106989	-5783.878002	-972.645024
TS-2(O1)	-5784.080301	-5783.856421	-972.6188626
INT-2(O1)	-5784.105762	-5783.877572	-972.6450872
TS-1(O2)	-5784.095224	-5783.868174	-972.6288245
INT-1(O2)	-5784.102134	-5783.872295	-972.6418608
TS-2(O2)	-5784.075497	-5783.851638	-972.6144684
INT-2(O2)	-5784.097391	-5783.869957	-972.6352836
CAT-OCH ₃	-5438.445713	-5438.315859	-626.8594283
TS-2-OCH ₃ (O1)	-5670.678522	-5670.459863	-859.1852112
INT-2-OCH ₃ (O1)	-5670.700623	-5670.479264	-859.2097244
TS-2-OCH ₃ (O2)	-5670.673141	-5670.454912	-859.1797031
INT-2-OCH ₃ (O2)	-5670.686286	-5670.464527	-859.1929613
CAT-NH ₂	-5379.259199	-5379.142567	-567.6600308
TS-2-NH ₂ (O1)	-5611.49448	-5611.290995	-799.9860845
INT-2-NH ₂ (O1)	-5611.515389	-5611.309121	-800.011118
TS-2-NH ₂ (O2)	-5611.482781	-5611.278537	-799.9762404
INT-2-NH ₂ (O2)	-5611.488688	-5611.280642	-799.9832936
CAT-CH ₃	-5363.217284	-5363.09189	-551.6088663
TS-2-CH ₃ (O1)	-5595.447434	-5595.234738	-783.9283601
INT-2-CH ₃ (O1)	-5595.468269	-5595.25243	-783.9531449

TS-2-CH₃(O2)	-5595.432913	-5595.21622	-783.9152377
INT-2-CH₃(O2)	-5595.43265	-5595.21656	-783.9147940
CAT-Ph	-5554.966432	-5554.793268	-743.4256402
TS-2-Ph(O1)	-5787.197004	-5786.933988	-975.7498863
INT-2-Ph(O1)	-5787.218722	-5786.953443	-975.7742403
TS-2-Ph(O2)	-5787.183144	-5786.919265	-975.7362579
INT-2-Ph(O2)	-5787.184586	-5786.918133	-975.7374108
CAT-CN	-5416.164727	-5416.065705	-604.5793295
TS-2-CN(O1)	-5648.407335	-5648.220591	-836.9099931
INT-2-CN(O1)	-5648.436085	-5648.247608	-836.9401335
TS-2-CN(O2)	-5648.395639	-5648.208428	-836.8995694
INT-2-CN(O2)	-5648.411976	-5648.220882	-836.9139547
CAT-F	-5423.18179	-5423.087493	-611.5848447
TS-2-F(O1)	-5655.421967	-5655.240099	-843.9135077
INT-2-F(O1)	-5655.446765	-5655.261614	-843.9398954
TS-2-F(O2)	-5655.417561	-5655.235517	-843.9109742
INT-2-F(O2)	-5655.439453	-5655.253686	-843.9314209
CAT-NMe₃	-5571.307657	-5571.129213	-759.7720321
TS-2-NMe₃(O1)	-5803.538429	-5803.271557	-992.0950144
INT-2-NMe₃(O1)	-5803.557732	-5803.287222	-992.1138841
TS-2-NMe₃(O2)	-5803.531606	-5803.264203	-992.0885304
INT-2-NMe₃(O2)	-5803.5567	-5803.286105	-992.1131127
CAT-PMe₃	-5857.920561	-5857.754301	-1046.432588
TS-2-PMe₃(O1)	-6090.145533	-6089.890173	-1278.748588
INT-2-PMe₃(O1)	-6090.156995	-6089.898418	-1278.758508
TS-2-PMe₃(O2)	-6090.14922	-6089.892687	-1278.755757
INT-2-PMe₃(O2)	-6090.176069	-6089.916648	-1278.782682
CAT-SMe₂	-5874.800006	-5874.670137	-1063.296135
TS-2-SMe₂(O1)	-6107.034135	-6106.814281	-1295.620475
INT-2-SMe₂(O1)	-6107.052608	-6106.829698	-1295.638818
TS-2-SMe₂(O2)	-6107.033597	-6106.812942	-1295.621413
INT-2-SMe₂(O2)	-6107.057368	-6106.83441	-1295.645733
CAT-C₂H₄	-5475.393663	-5475.281655	-663.8236889
TS-2-C₂H₄(O1)	-5707.626982	-5707.427285	-896.14836
INT-2-C₂H₄(O1)	-5707.647122	-5707.44529	-896.1681314
TS-2-C₂H₄(O2)	-5707.626816	-5707.426061	-896.1476207
INT-2-C₂H₄(O2)	-5707.654834	-5707.45126	-896.175052
CAT-C₂H₂	-5474.125229	-5474.039571	-662.5560578
TS-2-C₂H₂(O1)	-5706.360909	-5706.187304	-894.8810465
INT-2-C₂H₂(O1)	-5706.384245	-5706.207233	-894.9050673
TS-2-C₂H₂(O2)	-5706.359817	-5706.186638	-894.8794874
INT-2-C₂H₂(O2)	-5706.386424	-5706.210442	-894.9060437
CAT-NHC	-5701.683288	-5701.504893	-890.1888969

TS-2-NHC(O1)	-5933.907179	-5933.640027	-1122.503186
INT-2-NHC(O1)	-5933.918075	-5933.647799	-1122.514029
TS-2-NHC(O2)	-5933.91463	-5933.647104	-1122.512837
INT-2-NHC(O2)	-5933.936466	-5933.664954	-1122.534788
CH ₂ CHCN	-170.854084	-170.829311	-170.910621973
CH ₃ COOH	-229.1313765	-229.097269	-229.2006014
pre-COM	-5725.823443	-5725.603216	-914.3518055
TS-3	-5725.787733	-5725.575089	-914.3145143
INT-3	-5725.814274	-5725.596719	-914.3457366
TS-4	-5725.805109	-5725.587357	-914.3281823
INT-4	-5725.871608	-5725.652278	-914.3863716
TS-3'	-5725.812648	-5725.591929	-914.3381619
INT-3'	-5725.858443	-5725.635937	-914.380777
TS-4'	-5725.827030	-5725.608763	-914.3501169
INT-4'	-5725.83046683	-5725.611999	-914.3543672

Table S6.Imaginary frequencies (in cm⁻¹) of the transition states energies calculated at the B3LYP/DGDZVP level of theory in CH₂Cl₂ solvent

Names	I.F.	Names	I.F.
TS-1(O1)	-60.3 <i>i</i>	TS-1(O2)	-20.4 <i>i</i>
TS-2(O1)	-1244.7 <i>i</i>	TS-2(O2)	-1274.8 <i>i</i>
TS-2-OCH₃(O1)	-1336.1 <i>i</i>	TS-2-OCH₃(O2)	-1288.6 <i>i</i>
TS-2-NH₂(O1)	-1323.6 <i>i</i>	TS-2-NH₂(O2)	-1031.5 <i>i</i>
TS-2-CH₃(O1)	-1352.4 <i>i</i>	TS-2-CH₃(O2)	-187.0 <i>i</i>
TS-2-Ph(O1)	-1338.8 <i>i</i>	TS-2-Ph(O2)	-493.4 <i>i</i>
TS-2-CN(O1)	-1141.4 <i>i</i>	TS-2-CN(O2)	-1285.0 <i>i</i>
TS-2-F(O1)	-1232.5 <i>i</i>	TS-2-F(O2)	-1245.4 <i>i</i>
TS-2-NMe₃(O1)	-1310.3 <i>i</i>	TS-2-NMe₃(O2)	-1280.7 <i>i</i>
TS-2-PMe₃(O1)	-1209.9 <i>i</i>	TS-2-PMe₃(O2)	-1213.8 <i>i</i>
TS-2-SMe₂(O1)	-1323.5 <i>i</i>	TS-2-SMe₂(O2)	-1271.0 <i>i</i>
TS-2-C₂H₄(O1)	-1340.4 <i>i</i>	TS-2-C₂H₄(O2)	-1200.9 <i>i</i>
TS-2-C₂H₂(O1)	-1286.2 <i>i</i>	TS-2-C₂H₂(O2)	-1203.4 <i>i</i>
TS-2-NHC(O1)	-1195.3 <i>i</i>	TS-2-NHC(O2)	-1309.8 <i>i</i>
TS-3	-1310.6 <i>i</i>	TS-4	-308.8 <i>i</i>
TS-3'	-245.5 <i>i</i>	TS-4'	-443.5 <i>i</i>

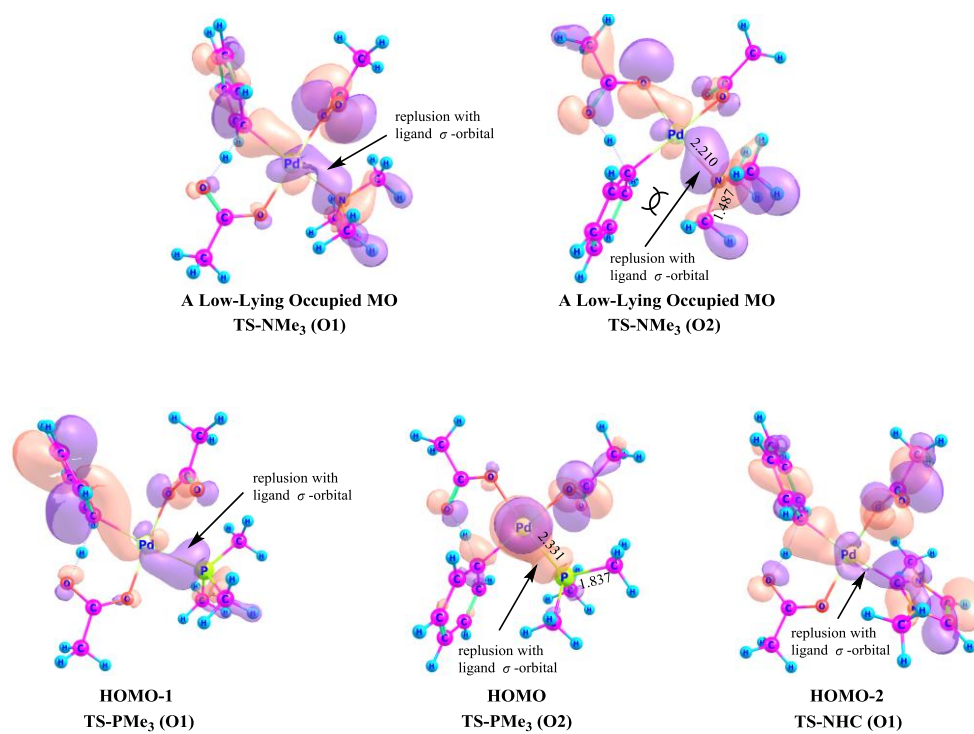


Figure S1. Some selected transition states and Kohn-Sham orbitals for the discussion on the role of neutral ligands